A SECOND-ORDER SCHEME WITH NONUNIFORM TIME STEPS
FOR A LINEAR REACTION-SUBDIFFUSION PROBLEM*

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Abstract. It is reasonable to assume that a discrete convolution structure dominates the local truncation error of any numerical Caputo formula because the fractional time derivative and its discrete approximation have the same convolutional form. We suggest an error convolution structure (ECS) analysis for a class of interpolation-type approximations to the Caputo fractional derivative. Our assumptions permit the use of adaptive time steps, such as is appropriate for accurately resolving the initial singularity of the solution and also certain complex behavior away from the initial time. The ECS analysis of numerical approximations has two advantages: (i) to localize (and simplify) the analysis of the approximation error of a discrete convolution formula on general nonuniform time grids; and (ii) to reveal the error distribution information in the long-time integration via the global consistency error. The core result in this paper is an ECS bound and a global consistency analysis of the nonuniform Alikhanov approximation, which is constructed at an offset point by using linear and quadratic polynomial interpolation. Using this result, we derive a sharp $L^2$-norm error estimate of a second-order Crank-Nicolson-like scheme for linear reaction-subdiffusion problems. An example is presented to show the sharpness of our analysis.

Key words. Caputo fractional derivative, nonuniform time mesh, error convolution structure, global consistency error, stability and convergence

AMS subject classifications. 65M06, 35B65

1. Introduction. The time-fractional diffusion equation provides a valuable tool for modeling complex systems such as glassy and disordered media [7]. This paper builds on our recent results [8, 9, 11] for the nonuniform mesh technique applied to the time discretization of the following reaction-subdiffusion problem in a bounded domain $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$),

\[
D_\alpha^t u - \Delta u = \kappa u + f(x, t) \quad \text{for } x \in \Omega \text{ and } 0 < t < T,
\]

\[
u = u_0(x) \quad \text{for } x \in \Omega \text{ when } t = 0,
\]

subject to the homogeneous Dirichlet boundary condition $u = 0$ on $\partial \Omega$. Here, the reaction coefficient $\kappa$ is a real constant, and $D_\alpha^t = C_0^t D_\alpha^t$ denotes the Caputo fractional derivative of order $\alpha$ ($0 < \alpha < 1$) with respect to time $t$, that is,

\[
(D_\alpha^t v)(t) := \int_0^t \omega_{1-\alpha}(t-s)v'(s) \, ds \quad \text{for } t > 0, \quad \text{where} \quad \omega_\beta(t) := t^{\beta-1}/\Gamma(\beta).
\]

1.1. Initial singularity and the nonuniform time meshes technique. In developing numerical methods for solving the subdiffusion problem (1.1), an important issue to be considered is that the solution $u$ is typically less regular than in the case of

*Submitted to the editors DATE.

Funding: This work was funded by NSFC grants 11771035, 91430216, U1530401; a grant 1008-56SYAH18037 from NUAA Scientific Research Starting Fund of Introduced Talent and a grant DRA2015518 from 333 High-level Personal Training Project of Jiangsu Province; Australian Research Council grant DP140101193.

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a classical parabolic PDE (as the limiting case $\alpha \to 1$). Sakamoto and Yamamoto [17] showed that if the initial data $v^0 \in H^2(\Omega) \cap H_0^1(\Omega)$, then the unique solution $u \in C^0([0,T];H^2(\Omega) \cap H_0^1(\Omega))$ and $\partial_t u \in L^2(\Omega)$. However, $\|\partial_t u(t)\|_{L^2(\Omega)} \leq C_u t^{\alpha-1}$ for $0 < t \leq T$, where the constant $C_u > 0$ is independent of $t$ but may depend on $T$. In fact, $u$ can only be a smooth function of $t$ if the initial data and source term satisfy some restrictive compatibility conditions [18].

The focus of this paper is on a second-order time discretization of (1.1). The spatial discretization is of less interest: we apply the standard Galerkin finite element method based on the weak form of the fractional PDE,

$$\langle D_t^\alpha u, v \rangle + \langle \nabla u, \nabla v \rangle = \kappa(u, v) + \langle f(t), v \rangle$$

for all $v \in H_0^1(\Omega)$ and for $0 < t \leq T$,

where $\langle u, v \rangle$ denotes the usual inner product in $L^2(\Omega)$. Thus, we construct the usual space of continuous, piecewise-linear functions with respect to a partition of $\Omega$ into subintervals (in 1D), triangles (in 2D) or tetrahedrons (in 3D) with the maximum diameter $h$, and let $X_h$ denote the subspace of functions satisfying the homogeneous Dirichlet boundary condition. In the usual way, (the semidiscrete) Galerkin finite element solution $u_h : [0,T] \to X_h$ is then defined by requiring that

$$\langle D_t^\alpha u_h, \chi \rangle + \langle \nabla u_h, \nabla \chi \rangle = \kappa(u_h, \chi) + \langle f(t), \chi \rangle$$

for all $\chi \in X_h$ and for $0 < t \leq T$,

with $u_h(0) = u_0 \approx u_0$ for a suitable $u_0 \in X_h$.

Consider (generally nonuniform) time levels $0 = t_0 < t_1 < t_2 < \cdots < t_N = T$ and define a fractional time level $t_{n-\theta} := \theta t_{n-1} + (1 - \theta)t_n$ for an off-set parameter $\theta \in [0,1/2)$. We denote the $k$th time-step size by $\tau_k := t_k - t_{k-1}$ for $1 \leq k \leq N$, and the maximum step size by $\tau := \max_{1 \leq k \leq N} \tau_k$. We also define the local step-size ratios

$$\rho_k := \frac{\tau_k}{\tau_{k+1}}$$

for $1 \leq k \leq N - 1$, and put $\rho := \max_{1 \leq k \leq N} \rho_k$.

For any time sequence $(v^k)_{k=0}^N$, define the backward difference $\nabla_\theta v^k := v^k - v^{k-1}$ and the interpolated value $v^{n-\theta} := \theta v^n + (1 - \theta)v^{n-1}$. We consider a numerical Caputo formula approximating $(D_t^\alpha v)(t_{n-\theta})$ of the form

$$\langle D_t^\alpha v^n, \chi \rangle + \langle \nabla v^n, \nabla \chi \rangle = \kappa(v^n, \chi) + \langle f(n-\theta), \chi \rangle$$

for appropriate discrete convolution kernels $A_{n-k}^{(n)}$. Our fully-discrete numerical solution, $u_h^n(\mathbf{x}) \approx u(\mathbf{x}, t_n)$ for $\mathbf{x} \in \Omega$, is then defined by a time-stepping scheme: we require that $u_h^n \in X_h$ satisfies

$$\langle (D_t^\alpha u_h)^n, \chi \rangle + \langle \nabla u_h^n, \nabla \chi \rangle = \kappa(u_h^n, \chi) + \langle f(t_{n-\theta}), \chi \rangle$$

for all $\chi \in X_h$ and for $1 \leq n \leq N$, with $u_h^0 = u_0$.

In the literature, several high-order numerical Caputo formulas have a discrete convolution form like (1.2), such as the L1-2 schemes [3, 10, 13] and the L2-1$\alpha$ formula [1, 12] that applied the piecewise quadratic polynomial interpolation. They achieve second-order temporal accuracy for sufficiently smooth solutions when applied to time approximation of the pure subdiffusion equation (1.1) with $\kappa = 0$. This article considers the L2-1$\alpha$ formula of Alikhanov [1], which employs a quadratic interpolant in each subinterval $[t_{k-1}, t_k]$ for $1 \leq k \leq n - 1$, and a linear interpolant in the final
subinterval \([t_{n-1}, t_{n-\theta}]\). The offset parameter is chosen as \(\theta = \alpha/2\) (in our notation). As described below, in the limit as \(\alpha \to 1\), this scheme reduces to the well-known Crank–Nicolson method \((\theta \to 1/2)\) for the classical diffusion equation. We therefore refer to the time-stepping scheme (1.3) as a fractional Crank–Nicolson method.

In the special case of uniform time steps \(\tau_n = \tau\), the discrete kernels \(A_n^{(n)} = A_{n-k}\) depend only on the difference \(n-k\), and were shown to be positive and monotonically decreasing, leading to a proof that the resulting fractional Crank–Nicolson scheme is stable and convergent of order \(O(\tau^2 + h^2)\) in the \(L_0\)-norm assuming that the solution \(u\) is sufficiently smooth [1]. However, as remarked above, in practice the time derivative \(\partial_t u\) typically behaves like \(O(\tau^{\alpha-1})\) as \(t \to 0\) [17, 18], and so this error bound breaks down.

In resolving a fixed singularity at \(t = 0\) of the type described above, a simple but useful technique to recover an optimal convergence order is to employ a smoothly graded mesh \(t_k = T(k/N)^\gamma\), where the grading parameter \(\gamma \geq 1\) is adapted to the strength of the singularity. The larger the value of \(\gamma\) the more strongly the mesh points are concentrated near \(t = 0\). Actually, such meshes have long been used in the numerical solution of Fredholm [4] and Volterra [2] integral equations, and their use for time-fractional PDEs is now well established [8, 10, 15, 19]. By using such a nonuniform mesh we will restore the second-order convergence in time of the fractional Crank–Nicolson scheme in [1] when the solution is not smooth at \(t = 0\). This idea was tested recently in [12] to resolve the initial singularity for the subdiffusion problem, corresponding to \(\kappa = 0\) in (1.1). However, this is only a part of our story.

We will establish the stability and convergence theory for the fractional Crank–Nicolson scheme on a wider class of nonuniform time meshes, not just the standard graded mesh described above. In this way, the theory could be applied in advanced studies on adaptive time grids required to resolve certain complex behavior (such as physical oscillations, blowup and so on) in nonlinear time-fractional PDEs. These goals are natural, at least for linear reaction-subdiffusion equations, since the backward Euler and Crank–Nicolson schemes for the linear parabolic equation are stable and convergent (provided \(\tau \to 0\)) on arbitrary nonuniform grids with \(\rho = O(1)\).

We refer the reader to other high-order time approximations in [6, 20] and the recent survey paper [5], which describes some useful approaches other than the nonuniform grids technique to achieve second-order accuracy in time.

### 1.2. Error convolution structure (ECS) analysis and a new problem.

Generally, our goals are theoretically challenging because the numerical Caputo formula always has a form of discrete convolutional summation (1.2). Actually, the consistency analysis over the whole time interval \([t_0, t_{n-\theta}]\) becomes too cumbersome to implement in practice when there has not enough grid information. To evade this difficulty, we propose an error convolution structure (ECS) analysis which begins by recasting the discrete Caputo formula (1.2) as

\[(D_\alpha v)^{n-\theta} = A_0^{(n)} v^n - \sum_{k=1}^{n-1} (\sum_{k=1}^{n} A_{n-k-1}^{(n)} - A_{n-k}^{(n)}) v^k - A_{n-1}^{(n)} v^0.\]

Consider the local truncation error \(\Upsilon^{n-\theta} := (D_\alpha v)(t_{n-\theta}) - (D_\alpha v)^{n-\theta}\). Given the construction of \((D_\alpha v)^{n-\theta}\) via local interpolation of \(v\), and provided the discrete convolution kernels \(A_k^{(n)}\) are decreasing, it is reasonable to conjecture that a discrete
convolution structure dominates the local truncation error:

\[(\text{ECS hypothesis}) \quad |\mathbf{Y}^n| \leq A_0^{(n)} G_{\text{loc}}^n + \sum_{k=1}^{n-1} (A_{n-k-1}^{(n)} - A_{n-k}^{(n)}) G_{\text{his}}^k.\]

Here, \(G_{\text{loc}}^n\) arises from the interpolation error on the local subinterval \([t_{n-1}, t_{n-\theta}]\) whereas the \(G_{\text{his}}^k\) \((1 \leq k \leq n-1)\) arise from the interpolation errors over the history \([t_0, t_{n-1}]\). Obviously, this ECS hypothesis localizes the consistency analysis of discrete Caputo formulas, and makes it possible to analyze the numerical approximations on a general class of nonuniform time grids.

Always, there is a loss of accuracy for \(\mathbf{Y}^n\) due to the initial singularity of \(\mathbf{Y}_{1-\theta}\). Actually, \(\mathbf{Y}_{1-\theta} = O(1)\) holds on any mesh and a superconvergence analysis should be required. For example, Stynes et al. [18, Lemma 5.2] showed that, on a graded mesh, the truncation error of the well-known L1 formula \((\theta = 0)\) behaves like \(\mathbf{Y}^n = O(n^{-\min\{2-\alpha, \gamma\alpha\}})\). Building on the ideas first introduced by Liao et al. [8, Section 3], we will prove a sharp error estimate via a fractional discrete Gronwall inequality (Theorem 1.1) that provides a global consistency error in the form

\[(1.5) \quad E_{\text{glob}}^n := \sum_{k=1}^{n} P^{(n)}_{n-k} |\mathbf{Y}^{k-\theta}|, \quad \text{for } 1 \leq k \leq n \leq N,
\]

where the complementary discrete convolution kernels \(P^{(n)}_{n-k}\) are chosen to enforce the identity

\[(1.6) \quad \sum_{j=k}^{n} P^{(n)}_{n-j} A^{(j)}_{j-k} \equiv 1 \quad \text{for } 1 \leq k \leq n \leq N.
\]

In fact, rearranging this identity yields a recursive formula (in effect, a definition)

\[(1.7) \quad P^{(n)}_0 := \frac{1}{A_0^{(n)}}, \quad P^{(n)}_{n-j} := \frac{1}{A_0^{(n)}} \sum_{k=j+1}^{n} (A^{(k)}_{k-j-1} - A^{(k)}_{k-j}) P^{(n)}_{n-k}, \quad 1 \leq j \leq n-1.
\]

In our recent paper [9], we showed that this approach is not limited to the L1 rule, but applies to a general class of discrete convolution kernels \(A^{(n)}_{n-k}\) satisfying the following two assumptions:

**A1.** There is a constant \(\pi_A > 0\) such that

\[A^{(n)}_{n-k} \geq \frac{1}{\pi_A t_k} \int_{t_{k-1}}^{t_k} \omega_{1-\alpha}(t_n - s) \, ds \quad \text{for } 1 \leq k \leq n \leq N;
\]

**A2.** The discrete kernels are monotone, \(A^{(n)}_{k-2} \geq A^{(n)}_{k-1} > 0\) for \(2 \leq k \leq n \leq N\).

In this case, the complementary kernels \(P^{(n)}_{n-k}\) in (1.7) are well-defined and non-negative, and satisfy [9, Lemma 2.1]

\[(1.8) \quad \sum_{j=1}^{n} P^{(n)}_{n-j} \omega_{1+(m-1)\alpha}(t_j) \leq \pi_A \omega_{1+m\alpha}(t_n) \quad \text{for } m = 0, 1 \text{ and } 1 \leq n \leq N.
\]
From the ECS hypothesis, one can exchange the order of summation to find
\[ \mathcal{E}_{\text{glob}}^n \leq \sum_{k=1}^{n} P_{n-k}^{(n)} A_0^{(k)} G_{\text{loc}}^k + \sum_{k=1}^{n} P_{n-k}^{(n)} \sum_{j=1}^{k-1} (A_{k-j-1}^{(k)} - A_{k-j}^{(k)}) G_{\text{his}}^j \]
\[ \leq \sum_{k=1}^{n} P_{n-k}^{(n)} A_0^{(k)} G_{\text{loc}}^k + \sum_{j=1}^{n-1} G_{\text{his}}^j \sum_{k=j+1}^{n} (A_{k-j-1}^{(k)} - A_{k-j}^{(k)}) P_{n-k}^{(n)} \]
and then, by using the definition (1.7) directly, arrive at
\[ (1.9) \quad \mathcal{E}_{\text{glob}}^n \leq \sum_{k=1}^{n} P_{n-k}^{(n)} A_0^{(k)} G_{\text{loc}}^k + \sum_{k=1}^{n-1} P_{n-k}^{(n)} A_0^{(k)} G_{\text{his}}^k. \]

Thus, by using the properties in (1.6) and (1.8), it is possible to obtain some useful error estimates on a variety of nonuniform grids, not limited to \( t_k = T(k/N) \).

Obviously, the first term on the right-hand side of (1.9) represents the total error contributions from discretization errors over the \( n \) current cells \([t_k, t_{k-\theta}]\) \((1 \leq k \leq n)\), whereas the second term represents those from discretization errors over the \( n(n-1) \) small cells in the historic intervals \([t_0, t_{k-1}]\) \((2 \leq k \leq n)\). This observation is very interesting: the local error in the current cell \([t_n, t_{n-\theta}]\) and the historic errors in the (long-time) interval \([t_0, t_{n-1}]\) make almost the same contribution, in the sense of convolutional summation, to the global consistency error of the discrete Caputo derivative. If some appropriate time grid is chosen to make \( G_{\text{his}}^k = O(G_{\text{loc}}^k) \) according to the error equidistribution principle, the error bound (1.9) becomes
\[ \mathcal{E}_{\text{glob}}^n \lesssim \sum_{k=1}^{n} P_{n-k}^{(n)} A_0^{(k)} G_{\text{loc}}^k. \]

It suggests that the global approximation error of the numerical Caputo formula (1.2) depends mainly on the local error \( G_{\text{loc}}^k \). In this sense, the error of numerical Caputo formula is “local” despite its overtly nonlocal nature.

**Table 1.1**

**Mesh restriction to stability for linear reaction-(sub)diffusion equations**

|               | backward Euler-like | Crank-Nicolson-like |
|---------------|---------------------|--------------------|
| diffusion \((\alpha \to 1)\)   | \( \rho = O(1) \)  | \( \rho = O(1) \)  |
| subdiffusion \((0 < \alpha < 1)\) | \( \rho = O(1) \)  | ?                  |

The ECS hypothesis plays a key role in our analysis. Actually, it has been used implicitly for the nonuniform L1 (fractional backward Euler-type) method employing a linear interpolant in each subinterval \([t_{k-1}, t_k]\) for \( 1 \leq k \leq n \). That analysis \([8, (3.9) \text{ in Lemma 3.3}] \) showed that the ECS hypothesis is valid for \( \rho = 1 \), or in other words provided \( \tau_k \leq \tau_{k+1} \) for all \( k \). In a further study \([11] \) on the two-level fast L1 scheme (which includes the original L1 scheme as a special case by setting the SOE approximation error \( \epsilon \equiv 0 \)), the ECS hypothesis is shown to be valid for any nonuniform mesh with \( \rho = O(1) \) \([11, \text{Lemma 3.1}] \), that is,
\[ |T^n| \leq a_0^{(n)} G^n + \sum_{k=1}^{n-1} (a_{n-k-1}^{(n)} - a_{n-k}^{(n)}) G^k. \]
where the L1 kernels $a_{n-k}^{(n)} := \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k} \omega_{1-\alpha}(t_n-s) \, ds$ for $1 \leq k \leq n$, and
\[
G^k := 2 \int_{t_{k-1}}^{t_k} (t-t_{k-1}) |v''(t)| \, dt \quad \text{for } 1 \leq k \leq n.
\]

This local step ratio restriction is the same as that for the backward Euler scheme for a classical diffusion equation. Considering Table 1.1, it is then natural to ask an elementary problem: what restriction on $\rho$ will suffice to ensure that the fractional Crank–Nicolson time-stepping scheme (1.3) is stable and convergent? We address this problem in the condition M1 below.

1.3. The discrete fractional Grönwall inequality and our answer. Our answer relies also on a discrete fractional Grönwall inequality suited to general nonuniform time meshes, proved in our recent paper [9, Theorem 3.1] and stated below (in a simplified form). This result involves the aforementioned discrete convolution kernels $F_{n-k}^{(n)}$, which are well-defined thanks to our assumptions A1–A2 on the discrete convolution kernels $A_{n-k}^{(n)}$ in the numerical Caputo formula (1.2). The Mittag–Leffler function $E_{\alpha}(z) := \sum_{k=0}^{\infty} z^k / \Gamma(1+k\alpha)$ also appears.

Theorem 1.1. Let the criteria A1–A2 hold, and the offset parameter $\theta \in [0, 1]$. Suppose that $\lambda > 0$ is a constant independent of the time steps and that the maximum time-step size
\[
\tau \leq 1 / \sqrt{2\Gamma(2-\alpha)\pi A \lambda}.
\]
If the non-negative time sequences $(\xi^k)_k^N$ and $(\nu^k)_k^N$ satisfy
\[
\sum_{k=1}^{n} A_{n-k}^{(n)} \frac{\nu^k}{\tau} \leq \lambda \left( \nu^{n-\theta} + \nu^{n-\theta} \xi^n \right) \quad \text{for } 1 \leq n \leq N,
\]
then the solution $(\nu^k)_k^N$ satisfies, for $1 \leq n \leq N$,
\[
\nu^n \leq 2E_{\alpha} \left( 2 \max(1, \rho) \pi_A \lambda t_n^\alpha \right) \left( \nu^0 + \max_{1 \leq k \leq n} \sum_{j=1}^{k} P_{k-j}^{(k)} \xi^j \right)
\]
\[
\leq 2E_{\alpha} \left( 2 \max(1, \rho) \pi_A \lambda t_n^\alpha \right) \left( \nu^0 + \pi_A \Gamma(1-\alpha) \max_{1 \leq j \leq n} \{ t_j^\alpha \xi^j \} \right).
\]

Thus, we need to complete the following three tasks:

**Task 1.** Verify the assumptions A1–A2 for the nonuniform Alikhanov kernels $A_{n-k}^{(n)}$ (defined in section 2) so that we can use the complementary kernels $P_{n-k}^{(n)}$ and apply the fractional Grönwall inequality to establish the stability of the fully discrete scheme (1.3).

**Task 2.** Verify the ECS hypothesis on nonuniform time meshes and determine the corresponding expressions for $G_{loc}^k$ and $G_{his}^k$ to insert in the bound (1.9) for the global consistency error $E_{\text{glob}}^n$.

**Task 3.** Establish a sharp error estimate in $L^2$ for the fully discrete scheme (1.3) for the subdiffusion problem (1.1) taking the initial singularity into account.

In more detail, we complete Task 1 in section 2. We describe the fractional Crank–Nicolson scheme and the corresponding discrete Alikhanov kernels $A_{n-k}^{(n)}$, and show in Theorem 2.2 (The lengthy and technical proofs for these properties of the discrete kernels $A_{n-k}^{(n)}$ are postponed until section 4) that the criteria A1–A2 hold given the following assumption on the mesh.
M1. The parameter $\theta = \alpha/2$, and the maximum time-step ratio is $\rho = 7/4$.

The special choice of $\theta$ in M1 is needed in any case to achieve second-order accuracy (see Remark 3.2). At the end of section 2, the discrete fractional Grönwall inequality is applied to establish stability for the time-stepping scheme (1.3). Actually, by showing that $e^\alpha = \|u_h^n\|$ satisfies (1.10), the a priori estimate with respect to initial and external perturbations in the forms (1.11)–(1.12), follows.

To verify the ECS hypothesis in Task 2 we make use of a proper lower bound for $A_n^{(n)} - A_n^{(n)}$, already proved in part (II) of Theorem 2.2 to ensure the criterion A2 directly. In the first part of section 3, an interpolation error formula for quadratic polynomials is derived in Lemma 3.3. Then we complete Task 2 in Theorem 3.4 by showing that the ECS hypothesis and the bound (1.9) for the global consistency error $e_{\text{glob}}$ are valid under the condition M1.

Task 3 is completed in the second part of section 3. To make our analysis extendable (such as, for distributed-order subdiffusion problems), we assume that there is a constant $C_u > 0$ such that the continuous solution $u$ satisfies

$$\|u^{(l)}(t)\|_{H^2(\Omega)} \leq C_u (1 + t^{\alpha-l})$$

for $l = 0, 1, 2, 3$, and $0 < t \leq T$,

where $\sigma \in (0, 1) \cup (1, 2)$ is a regularity parameter. For example [14, 17, 19], the assumption (1.13) holds with $\sigma = \alpha$ for the subdiffusion problem (1.1) if $f(x, t) = 0$ and $u_0 \in H^2(\Omega) \cap H^2(\Omega)$. To resolve such a solution $u$ efficiently, it is appropriate to choose the time mesh in such a way that the following condition [2, 16] holds.

M2. There is a constant $C_\gamma > 0$ such that $\tau_k \leq C_\gamma \tau \min\{1, t_k^{1-1/\gamma}\}$ for $1 \leq k \leq N$, with $t_k \leq C_\gamma t_{k-1}$ and $\tau_k / t_k \leq C_\gamma \tau_{k-1} / t_{k-1}$ for $2 \leq k \leq N$.

Here, the parameter $\gamma > 0$ controls the extent to which the time levels are concentrated near $t = 0$. If the mesh is quasi-uniform, then M2 holds with $\gamma = 1$. As $\gamma$ increases, the initial step sizes become smaller compared to the latter ones. A simple example of a family of meshes satisfying M2 is the graded mesh $t_k = T(k/N)^\gamma$.

When the offset parameter $\theta = 0$ and (1.2) is the nonuniform L1 method, our previous work [8, Theorem 3.1] proved the following error bound for the fully discrete scheme (1.3),

$$\|u(t_n) - u_h^n\| \leq \frac{C_u}{\sigma(1 - \alpha)} \tau^{\min(\gamma \sigma, 2)} + C_u h^2, \quad 1 \leq n \leq N.$$}

In particular, the error is of order $O(\tau^{\gamma \sigma} + h^2)$ if $\gamma \geq (2 - \alpha)/\sigma$. When $\theta = \alpha/2$ and (1.2) is the Alikhanov formula, Theorem 3.9 establishes an error bound

$$\|u(t_n) - u_h^n\| \leq \frac{C_u}{\sigma(1 - \alpha)} \tau^{\min(\gamma \sigma, 2)} + C_u h^2, \quad 1 \leq n \leq N,$$

which is of order $O(\tau^{\gamma} + h^2)$ if $\gamma \geq 2/\sigma$. Thus, in comparison to the L1 scheme, the Alikhanov formula leads to a higher convergence rate with respect to $\tau$; however, both methods achieve only order $O(\tau^\alpha + h^2)$ convergence on a uniform mesh. Numerical experiments in section 5 confirm that our error bound (1.14) is sharp.

2. Numerical Caputo formula and stability. Let $\Pi_{1,k} v$ denote the linear interpolant of a function $v$ with respect to the nodes $t_{k-1}$ and $t_k$, and let $\Pi_{2,k} v$ denote the quadratic interpolant with respect to $t_{k-1}$ and $t_k$. The corresponding interpolation errors are denoted by

$$(\Pi_{p,k} v)(t) := v(t) - (\Pi_{p,k} v)(t) \quad \text{for} \quad p \in \{1, 2\}.$$
Recalling that $\rho_k = \tau_k/\tau_{k+1}$, it is easy to find (for instance, by using the Newton forms of the interpolating polynomials) that

$$\langle \Pi_{1,k} v \rangle'(t) = \frac{\nabla_\tau v^k}{\tau_k} \quad \text{and} \quad \langle \Pi_{2,k} v \rangle'(t) = \frac{\nabla_\tau v^k}{\tau_k} + \frac{2(t-t_{k-1/2})}{\tau_k(\tau_k + \tau_{k+1})} (\rho_k \nabla_\tau v^{k+1} - \nabla_\tau v^k).$$

Throughout this paper, we will always use the notation

$$\varpi_n(t) := -\omega_{2-\alpha}(t_{n-\theta} - t) \leq 0 \quad \text{for} \quad 0 \leq t \leq t_{n-\theta}. $$

If $0 \leq t < t_{n-\theta}$, then $\varpi_n'(t) = \omega_{1-\alpha}(t_{n-\theta} - t) > 0$, $\varpi_n''(t) = -\omega_{-\alpha}(t_{n-\theta} - t) > 0$ and $\varpi_n'''(t) = \omega_{-\alpha-1}(t_{n-\theta} - t) > 0$

2.1. Discrete Caputo formula. The nonuniform Alikhanov approximation to the Caputo derivative $(D_\tau^\alpha v)(t_{n-\theta})$ is defined by

$$\left(D_\tau^\alpha v\right)^{n-\theta} := \int_{t_{n-1}}^{t_{n-\theta}} \varpi_n(s) \left(\Pi_{1,n} v\right)'(s) \, ds + \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \varpi_n(s) \left(\Pi_{2,k} v\right)'(s) \, ds$$

$$= a_0^{(n)} \nabla_\tau v^n + \sum_{k=1}^{n-1} \left(a_{n-k}^{(n)} \nabla_\tau v^k + \rho_k b_{n-k}^{(n)} \nabla_\tau v^{k+1} - b_{n-k}^{(n)} \nabla_\tau v^k\right),$$

where the discrete coefficients $a_{n-k}^{(n)}$ and $b_{n-k}^{(n)}$ are defined by

$$a_{n-k}^{(n)} := \frac{1}{\tau_k} \int_{t_{k-1}}^{\min\{t_k, t_{n-\theta}\}} \varpi_n(s) \, ds, \quad 1 \leq k \leq n;$$

$$b_{n-k}^{(n)} := \frac{2}{\tau_k(\tau_k + \tau_{k+1})} \int_{t_{k-1}}^{t_k} (s-t_{k-1}) \varpi_n(s) \, ds, \quad 1 \leq k \leq n-1.$$

When $\theta = 0$, the coefficients $a_{n-k}^{(n)}$ in (2.2) are just the discrete convolution kernels in the L1 formula [8]. Notice that if $\alpha \to 1$, then $\omega_{2-\alpha}(t) \to 1$ whereas $\omega_{1-\alpha}(t) \to 0$, uniformly for $t$ in any compact subinterval of the open half-line $(0, \infty)$. Thus,

$$a_0^{(n)} = \omega_{2-\alpha}(1-\theta)/\tau_n \to 1/\tau_n$$

whereas $a_{n-k}^{(n)} \to 0$ and $b_{n-k}^{(n)} \to 0$ for $1 \leq k \leq n-1$. It follows that $(D_\tau^\alpha v)^{n-\theta} \to \nabla_\tau v^n/\tau_k$ and $\theta = \alpha/2 \to 1/2$ so the scheme (1.3) tends to the Crank–Nicolson method for a linear parabolic equation. This is why we also call (1.3) a fractional Crank–Nicolson time-stepping method.

Rearranging the terms in (2.1), we obtain the compact form (1.2) where the discrete convolution kernels $A_{n-k}^{(n)}$ are defined as follows: $A_{0}^{(1)} := a_0^{(1)}$ if $n = 1$ and, for $n \geq 2$,

$$A_{n-k}^{(n)} := \begin{cases} a_0^{(n)} + \rho_{n-1} b_1^{(n)}, & \text{for } k = n, \\ a_{n-k}^{(n)} + \rho_k b_{n-k}^{(n)} - b_{n-k}^{(n)}, & \text{for } 2 \leq k \leq n-1, \\ a_{n-1}^{(n)} - b_{n-1}^{(n)}, & \text{for } k = 1. \end{cases}$$

Before studying the kernels $A_{n-k}^{(n)}$, we present two alternative formulas for $b_{n-k}^{(n)}$. Recall the integral form of error term for the trapezoidal rule, which can be derived by the Taylor expansion with the integral remainder. Integration by parts yields the following identities.
Lemma 2.1. For any function \( q \in C^2([t_{k-1}, t_k]) \),
\[
\int_{t_{k-1}}^{t_k} (s - t_{k-1}/2) q'(s) \, ds = - \int_{t_{k-1}}^{t_k} \left( \Pi_{1,k} q \right)(s) \, ds \\
= \frac{1}{2} \int_{t_{k-1}}^{t_k} (s - t_{k-1})(t_k - s) q''(s) \, ds.
\]

Taking \( q := \varpi_n \) in Lemma 2.1, the definition (2.3) of \( b_{n-k}^{(n)} \) gives
\[(5) \quad b_{n-k}^{(n)} = -2 \int_{t_{k-1}}^{t_k} \frac{(\Pi_{1,k} \varpi_n)(s)}{\tau_k(\tau_{k+1} + \tau_k)} \, ds \\
= \int_{t_{k-1}}^{t_k} \frac{(t_k - s)(s - t_{k-1})}{\tau_k(\tau_{k+1} + \tau_k)} \varpi_n''(s) \, ds, \quad 1 \leq k \leq n - 1.
\]

The following theorem gathers some useful properties of the discrete kernels \( A_{n-k}^{(n)} \), but the rigorous proof is left to section 4. It should be noted here that this proof is quite different from the previous analysis \([1, 3, 13]\) for the discrete convolution kernels in high-order numerical Caputo formulas with uniform time-steps.

Theorem 2.2. Let \( M1 \) hold and consider the discrete kernels defined in (2.4).

(I) The discrete kernels \( A_{n-k}^{(n)} \) are bounded,
\[A_0^{(n)} \leq \frac{24}{11T_n} \int_{t_{n-1}}^{t_n} \omega_1^{\alpha}(t_n - s) \, ds\]
and
\[A_{n-k}^{(n)} \geq \frac{4}{11T_k} \int_{t_{k-1}}^{t_k} \omega_1^{\alpha}(t_n - s) \, ds, \quad 1 \leq k \leq n;\]

(II) The discrete kernels \( A_{n-k}^{(n)} \) are monotone,
\[A_{n-k-1}^{(n)} - A_{n-k}^{(n)} \geq (1 + \rho_k)b_{n-k}^{(n)} + \frac{1}{5\tau_k} \int_{t_{k-1}}^{t_k} (t_k - s) \varpi_n''(s) \, ds, \quad 1 \leq k \leq n - 1;\]

(III) And the first kernel \( A_0^{(n)} \) is appropriately larger than the second one,
\[\frac{1 - 2\theta}{1 - \theta} A_0^{(n)} - A_1^{(n)} > 0 \quad \text{for} \ n \geq 2.
\]

The first part (I) implies that the criterion \( A1 \) holds with \( \pi_A = \frac{1}{11} \), the second part (II) ensures that the criterion \( A2 \) is valid and the third part (III) is used to prove the following corollary. These results allow us to apply Theorem 1.1 and establish the stability of the time-stepping scheme (1.3). Also, the second part (II) establishes a stronger estimate used in obtaining an ECSE bound for the error analysis (see Theorem 3.4).

Corollary 2.3. Under the condition \( M1 \), the discrete Caputo formula (1.2) with the discrete kernels (2.4) satisfies
\[\langle \mathcal{D}_\theta^n v^{n-\theta}, v^{n-\theta} \rangle \geq \frac{1}{2} \sum_{k=1}^{n} A_{n-k}^{(n)} \| v^k \|^2 \quad \text{for} \ 1 \leq n \leq N.
\]
Proof. The inequality is known to hold [9, Lemma 4.1] provided $A2$ is satisfied and $\theta(n) \geq \theta$ for $1 \leq n \leq N$, where

$$\theta(1) = \frac{1}{2} \quad \text{and} \quad \theta(n) = \frac{A_0^{(n)} - A_1^{(n)}}{2A_0^{(n)} - A_1^{(n)}} \quad \text{for } n \geq 2.$$ 

Obviously, Theorem 2.2 (II) ensures that $A2$ holds, and the condition $M1$ leads to $\theta(1) \geq \theta$. From Theorem 2.2 (III), $\theta(n) \geq \theta$ holds also for $n \geq 2$. \hfill $\Box$

2.2. Unconditional stability. By taking the $\chi = u_h^{n-\theta}$ in (1.3), one has

$$\langle (D^\alpha_t u_h)^{n-\theta}, u_h^{n-\theta} \rangle \leq \kappa_+ \|u_h^{n-\theta}\|^2 + \langle f(t_n-\theta), u_h^{n-\theta} \rangle \quad \text{for } 1 \leq n \leq N,$$

where $\kappa_+ := \max(\kappa, 0)$ and the property $\langle \nabla u_h^{n-\theta}, \nabla u_h^{n-\theta} \rangle \geq 0$ was used. Therefore, applying the above Corollary 2.3 along with the Cauchy–Schwarz and triangle inequalities, one gets

$$\sum_{k=1}^n A_{n-k}^{(n)} \langle \|u_h^k\|^2 \rangle \leq 2\kappa_+ \left((1-\theta)\|u_h^n\| + \theta\|u_h^{n-1}\|\right)^2$$

$$+ 2\left((1-\theta)\|u_h^n\| + \theta\|u_h^{n-1}\|\right)\|f(t_n-\theta)\|, \quad 1 \leq n \leq N,$$

which has the form of (1.10) with

$$\lambda := 2\kappa_+, \quad \nu^k := \|u^k\| \quad \text{and} \quad \xi^k := 2\|f^{k-\theta}\| \quad \text{for } 1 \leq k \leq N.$$ 

Note that Theorem 2.2 shows the criteria $A1$–$A2$ of Theorem 1.1 are satisfied with $\pi_A = 11/4$, and the condition $M1$ gives $\rho = 7/4$. Therefore, applying Theorem 1.1, we see that the time-stepping method (1.3) is stable in the following sense.

**Theorem 2.4.** If $M1$ holds with the maximum time step $\tau \leq 1/\sqrt{\Pi(2-\alpha)\kappa_+}$ (there is no limit to the maximum time step if $\kappa \leq 0$), then the solution $u^n$ of the time-stepping scheme (1.3) is stable, that is,

$$\|u_h^n\| \leq 2E_0(20\kappa_+t_n^\alpha) \left(\|u_{0h}\| + 2 \max_{1 \leq k \leq n} \sum_{j=1}^k \|f(t_{j-\theta})\|\right)$$

$$\leq 2E_0(20\kappa_+t_n^\alpha) \left(\|u_{0h}\| + 6\Gamma(1-\alpha) \max_{1 \leq j \leq n} \left\{t_j^\alpha \|f(t_{j-\theta})\|\right\}\right) \quad \text{for } 1 \leq n \leq N.$$ 

3. Global consistency error and convergence. We now derive a representation for the consistency error of the discrete Caputo derivative (1.2) with the discrete kernels in (2.4). Fix a function $v(t)$ and decompose the local consistency error into $n$ terms corresponding to the $n$ subintervals, writing

$$\Upsilon^{n-\theta} := (D^\alpha_t v)(t_{n-\theta}) - (D^\alpha_t v)^{n-\theta} = \sum_{k=1}^n \Upsilon_k^{n-\theta}, \quad 1 \leq n \leq N,$$

where, recalling the notations $\varpi_n(s)$, $\widetilde{\Pi}_{1,k}v$ and $\widetilde{\Pi}_{2,k}v$ from section 2,

$$\Upsilon_k^{n-\theta} := \int_{t_{k-1}}^{t_k} \varpi(s)(\widetilde{\Pi}_{2,k}v)'(s) \, ds, \quad 1 \leq k \leq n - 1 \leq N - 1,$$

$$\Upsilon_n^{n-\theta} := \int_{t_{n-1}}^{t_n} \varpi(s)(\widetilde{\Pi}_{1,n}v)'(s) \, ds, \quad 1 \leq n \leq N.$$
Theorem 2.4 suggests that one can consider the global

\[ (3.6) \quad \forall n, \quad \int_{t_{n-1}}^{t_n} (s - t_{n-1})^2 |\varphi'''(s)| \, ds + \frac{3}{2} \int_{t_{n-1}}^{t_n} (t_n - s) |\varphi'''(s)| \, ds, \]

and the following quantities

\[ (3.7) \quad \forall n, \quad \int_{t_{n-1}}^{t_n} (t_n - s)^2 |\varphi'''(s)| \, ds + \frac{3}{2} \int_{t_{n-1}}^{t_n} (s - t_{n-1})^2 |\varphi'''(s)| \, ds, \]

assuming in what follows that \( \varphi \) is such that these integrals exist and are finite.

**3.1. Global consistency error.**

**Lemma 3.1.** For any function \( \varphi \in C^3((0,T]) \), the local consistency error \( \Upsilon_n^{-\theta} \) in (3.3) satisfies

\[ |\Upsilon_n^{-\theta}| \leq a_0^n G_{\text{loc}}^n \leq A_0^n G_{\text{loc}}^n \quad \text{for } 1 \leq n \leq N. \]

**Proof.** Taylor expansion (with integral remainder) about \( t_{n-1/2} \) shows that

\[ \varphi'(s) = \varphi'(t_{n-1/2}) + \varphi''(t_{n-1/2})(s - t_{n-1/2}) + \int_{t_{n-1/2}}^{s} (s - y) \varphi'''(y) \, dy, \]

and

\[ (\Pi_1 \varphi)'(s) = \varphi''(t_{n-1/2})(s - t_{n-1/2}) + \int_{t_{n-1/2}}^{s} (s - y) \varphi'''(y) \, dy, \]

\[ - \frac{1}{2 \tau_n} \int_{t_{n-1}}^{t_{n-1/2}} (y - t_{n-1})^2 \varphi'''(y) \, dy - \frac{1}{2 \tau_n} \int_{t_{n-1/2}}^{t_n} (t_n - y)^2 \varphi'''(y) \, dy. \]

Inserting these four terms in (3.3) yields the splitting \( \Upsilon_n^{-\theta} = \sum_{\ell=1}^{4} \Upsilon_{n,\ell}^{-\theta} \). After integrating by parts, we find that

\[ \Upsilon_{n,1}^{-\theta} = (\alpha - 2 \theta) \frac{(1 - \theta)^{1-\alpha}}{2 \Gamma(3-\alpha)} \varphi''(t_{n-1/2}) \tau_n^{2-\alpha}, \]

which vanishes for \( \theta = \alpha / 2 \). For the term \( \Upsilon_{n,2}^{-\theta} \), we split the integration interval \([t_{n-1}, t_{n-\theta}]\) into two parts: \([t_{n-1}, t_{n-1/2}]\) and \([t_{n-1/2}, t_{n-\theta}]\). Since \( t_{n-1/2} < t_{n-\theta} < t_n \), the second term reads

\[ \Upsilon_{n,2}^{-\theta} = \int_{t_{n-1}^{-1/2}}^{t_n} \varphi'(s) \int_{t_{n-1/2}}^{s} (s - y) \varphi'''(y) \, dy \, ds \]

\[ = \int_{t_{n-1}}^{t_{n-1/2}} \varphi'(s) \int_{t_{n-1/2}}^{s} (s - y) \varphi'''(y) \, dy \, ds + \int_{t_{n-1/2}}^{t_n} \varphi'(s) \int_{t_{n-1/2}}^{s} (s - y) \varphi'''(y) \, dy \, ds. \]

Reversing the order of integration, then integrating by parts in the second term and using \( \varphi(t_{n-\theta}) = 0 \), we have

\[ \Upsilon_{n,2}^{-\theta} = \int_{t_{n-1}}^{t_{n-1/2}} \varphi'''(y) \int_{t_{n-1}}^{y} (y - s) \varphi'(s) \, ds \, dy + \int_{t_{n-1/2}}^{t_n} \varphi'''(y) \int_{t_{n-1/2}}^{y} (s - y) \varphi'(s) \, ds \, dy \]

\[ = \int_{t_{n-1}}^{t_{n-1/2}} \varphi'''(y) \int_{t_{n-1}}^{y} (y - s) \varphi'(s) \, ds \, dy - \int_{t_{n-1/2}}^{t_n} \varphi'''(y) \int_{t_{n-1/2}}^{y} \varphi'(s) \, ds \, dy. \]
The inner integrals can be estimated as
\[
\left| \int_{t_n-\theta}^{t_n} \varpi_n(s) \, ds \right| \leq \varpi_n(t_{n-1}) \left( t_n - t_{n-1} \right)^2 / 2 \quad \text{for } t_{n-1} < y < t_{n-1}/2,
\]
\[
\left| \int_y^{t_n-\theta} \varpi_n(s) \, ds \right| \leq \varpi_n(t_{n-1}/2) \left( t_n - y \right) \quad \text{for } t_{n-1}/2 < y < t_n - \theta.
\]

Recalling the definition (2.2) of \(a_0^{(n)}\), we see that \(\omega_{2-\alpha}(t_n - t_{n-1}) = \tau_n a_0^{(n)}\) and then
\[
\varpi_n(t_{n-1}/2) = \omega_{2-\alpha}(t_n - t_{n-1}) \leq \omega_{2-\alpha}(t_n - t_{n-1}) = \tau_n a_0^{(n)},
\]
\[
\varpi_n'(t_{n-1}/2) = \omega_{1-\alpha}(t_n - t_{n-1}) = 2 \tau_n \omega_{2-\alpha}(t_n - t_{n-1}/2) \leq 2 a_0^{(n)},
\]
where we used the fact that \(t_n - t_{n-1}/2 = (1 - \alpha) \tau_n/2\). Hence, it follows that
\[
\left| \Upsilon_{n,2}^{n-\theta} \right| \leq a_0^{(n)} \int_{t_{n-1}}^{t_{n-1}/2} (y - t_{n-1})^2 |v''(y)| \, dy + a_0^{(n)} \tau_n \int_{t_{n-1}/2}^{t_n} (t_n - y) |v''(y)| \, dy,
\]
and finally
\[
\sum_{\ell=3}^{4} \Upsilon_{n,\ell}^{n-\theta} \leq \frac{a_0^{(n)}}{2} \int_{t_{n-1}}^{t_{n-1}/2} (y - t_{n-1})^2 |v''(y)| \, dy + \frac{a_0^{(n)}}{2} \int_{t_{n-1}/2}^{t_n} (t_n - y)^2 |v''(y)| \, dy.
\]

Thus the triangle inequality yields \(\left| \Upsilon_{n}^{n-\theta} \right| \leq a_0^{(n)} G_{local}^n \) where \(G_{local}^n \) is defined in (3.4). The definition (2.4) implies \(a_0^{(n)} \leq A_0^{(n)}\) and completes the proof.

Remark 3.2. If we were to choose \(\theta \neq \alpha/2\), the term (3.6) would limit the consistency error to an order of \(O(\tau_n^{2-\alpha})\), even for smooth solutions.

To estimate the remaining terms in (3.2), we present an interpolation error formula for the quadratic polynomial \(I_{2,k}v\) employed in the Alikhanov formula (1.2), but leave the proof to Appendix A. This formula is crucial for verifying the ECS hypothesis for the local consistency error \(\Upsilon^{n-\theta}\).

Lemma 3.3. If \(v \in C^3([t_{k-1}, t_{k+1}])\) and \(q \in C^2([t_{k-1}, t_k])\), then
\[
\int_{t_{k-1}}^{t_k} q'(t) \widetilde{I}_{2,k}v'(t) \, dt = \int_{t_{k-1}}^{t_{k+1}} \left( t_{k+1} - s \right)^2 v''(s) \, ds \int_{t_{k-1}}^{t_k} \frac{\widetilde{I}_{2,k}q(t) \, dt}{(\tau_{k+1} + \tau_k)\tau_{k+1}}
\]
\[
- \int_{t_{k-1}}^{t_k} \left( s - t_{k-1} \right)^2 v''(s) \, ds \int_{t_{k-1}}^{t_k} \frac{\widetilde{I}_{2,k}q(t) \, dt}{(\tau_{k+1} + \tau_k)\tau_k}
\]
\[
+ \int_{t_{k-1}}^{t_k} v''(s) \, ds \int_{t_{k-1}}^{t_k} (\widetilde{I}_{2,k}q(t) \, dt), \quad 1 \leq k \leq n - 1.
\]

Theorem 3.4. Assume that the mesh condition M1 holds and \(v \in C^3((0,T])\). For the nonuniform Alikhanov formula (1.2) with the discrete kernels (2.4), an ECS dominates the local consistency error \(\Upsilon^{n-\theta}\) in (3.1), that is,
\[
\left| \Upsilon_{n}^{n-\theta} \right| \leq A_0^{(n)} G_{loc}^n + \sum_{k=1}^{n-1} (A_{n-k-1}^{(n)} - A_{n-k}^{(n)}) G_{hists}^k \quad \text{for } 1 \leq n \leq N,
\]
and consequently the global consistency error satisfies

\[ E_{\text{glob}}^n \leq \sum_{k=1}^{n} P_{n-k}^{(n)} \varepsilon_{\text{loc}}^{(k)} G_{\text{loc}}^{k} + \sum_{k=1}^{n-1} P_{n-k}^{(n)} \varepsilon_{\text{his}}^{(k)} G_{\text{his}}^{k} \quad \text{for } 1 \leq n \leq N, \]

where \( G_{\text{loc}}^{k} \) and \( G_{\text{his}}^{k} \) are defined by (3.4) and (3.5), respectively.

**Proof.** According to the arguments in subsection 1.2, it suffices to verify the first inequality (the ECS bound). The definition (??) of \( Y_{k}^{n-\theta} \) and Lemma 3.3 (taking \( q := \varpi_n \)) yield

\[
Y_{k}^{n-\theta} = \frac{b_{n-k}^{(n)}}{2} \int_{t_{k-1}}^{t_k} (s - t_{k-1})^2 v'''(s) \, ds - \frac{\rho_k b_{n-k}^{(n)}}{2} \int_{t_{k+1}}^{t_{k+1}} (t_{k+1} - s)^2 v'''(s) \, ds \\
+ \int_{t_{k-1}}^{t_k} v'''(s) \int_{t_{k-1}}^{s} (\Pi_{1,k} \varpi_n(t)) \, dt \, ds, \quad 1 \leq k \leq n - 1,
\]

where the alternative definition (2.5) of \( b_{n-k}^{(n)} \) has been used. Recall the error formula of linear interpolation [8, Lemma 3.1],

\[
(\Pi_{1,k} \varpi_n)(t) = \int_{t_{k-1}}^{t_k} \chi_k(t, s) \varpi_n'(s) \, ds, \quad t_{k-1} < t < t_k, \quad 1 \leq k \leq n - 1,
\]

where the Peano kernel \( \chi_k(t, s) = \max \{t - y, 0\} - (t - t_{k-1})(t_k - y)/\tau_k \) satisfies

\[
-\frac{t - t_{k-1}}{\tau_k} (t_k - y) \leq \chi_k(t, y) < 0 \quad \text{for any } t, y \in (t_{k-1}, t_k).
\]

The inner integral in the last term of (3.7) can be bounded by

\[
\left| \int_{t_{k-1}}^{s} (\Pi_{1,k} \varpi_n(t)) \, dt \right| \leq \frac{1}{2} (s - t_{k-1})^2 \int_{t_{k-1}}^{t_k} \frac{t_k - s}{\tau_k} \varpi_n''(s) \, ds, \quad t_{k-1} < s < t_k.
\]

By the definition (3.5) of \( G_{\text{his}}^{n} \) and the triangle inequality, we obtain from (3.7) that

\[
|Y_{k}^{n-\theta}| \leq \frac{1}{5} \left( (1 + \rho_k)b_{n-k}^{(n)} + \int_{t_{k-1}}^{t_k} \frac{t_k - s}{\tau_k} \varpi_n''(s) \, ds \right) G_{\text{his}}^{k} \leq (A_{n-k-1}^{(n)} - A_{n-k}^{(n)}) G_{\text{his}}^{k},
\]

where Theorem 2.2 (II) was used in the second inequality. Then the definition (3.1) and Lemma 3.1 yield the first inequality immediately. The proof is completed. \( \square \)

**Remark 3.5.** Traditionally, the global approximation error would be estimated by using the truncation error \( Y^{n-\theta} \) directly. Once an upper bound of \( |Y^{n-\theta}| \) is available, the inequality (1.8) with \( m = 0 \) will give the global approximate error

\[
E_{\text{glob}}^n \leq \sum_{j=1}^{n} P_{n-j}^{(n)} \omega_1(\alpha) \left( \max_{1 \leq i \leq n} \varpi_1(\alpha) \right) \leq \pi \Gamma(1 - \alpha) \max_{1 \leq i \leq n} t_i^\alpha |Y_i^{n-\theta}|.
\]

Nonetheless, the local and global consistency errors described in Theorem 3.4 present a new understanding of the error contributions generated by the two different polynomial approximations, respectively, in the local cell \([t_{n-1}, t_{n-\theta}]\) and the historical interval \([0, t_{n-1}]\) of the fractional Caputo derivative.
Originally, our ECS bound for $\Upsilon^{n-\theta}$ is constructed to preserve the convolution structure of the Caputo fractional derivative as much as possible. A direct estimate of the global consistency error (1.5) would lead to the double sum $\sum_{k=1}^{n} \sum_{j=1}^{n} |\Upsilon_{j}^{k-\theta}|$, whereas the ECS bound leads to a single sum $\sum_{k=1}^{n} P_{n-k} A_{0}^{(k)} (G_{\text{loc}}^{k} + G_{\text{his}}^{k})$. This simplification assists for proving sharp error bounds even with quite general nonuniform meshes. Nonetheless, an explicit bound for the complementary discrete kernel $P_{n-j}^{(n)}$ remains an open problem until now, and we will make full use of the identity (1.6) and the upper bound (1.8) in the subsequent analysis.

**Lemma 3.6.** Assume that $v \in C^{2}([0, T])$, and there exists a positive constant $C_{v}$ such that $|v'''(t)| \leq C_{v}(1 + t^{\sigma - 3})$ for $0 < t \leq T$, where $\sigma \in (0, 1) \cup (1, 2)$ is a regularity parameter. If the mesh condition M1 holds, for $1 \leq n \leq N$, then the global consistency error satisfies

$$E_{\text{glob}}^{n} \leq C_{v} \left( \tau_{n}^{2} / \sigma + t_{1}^{\sigma - 3} \tau_{n}^{3} \right) + \frac{1}{1 - \alpha} \max_{2 \leq k \leq n} \frac{t_{n-k}^{2} t_{k-1}^{\sigma - 3} \tau_{n}^{3}}{\tau_{k-1}}.$$  

**Proof.** The bounds on the discrete kernel $A_{n-k}^{(n)}$ in Theorem 2.2 (I) yield the inequalities

$$A_{0}^{(k)} \leq \frac{24}{11} \omega_{2-\alpha}(\tau_{k}) / \tau_{k}, \quad A_{k-2}^{(k)} \geq \frac{4}{11} \omega_{1-\alpha}(t_{k} - t_{1}),$$

and

$$A_{0}^{(k)} < \frac{6 \omega_{2-\alpha}(\tau_{k})}{\tau_{k} \omega_{1-\alpha}(t_{k} - t_{1})} \leq \frac{6}{1 - \alpha} \frac{(t_{k} - t_{1})^{\alpha}}{\tau_{k}}, \quad 2 \leq k \leq n.$$  

Furthermore, the identity (1.6) for the complementary discrete kernel $P_{n-j}^{(n)}$ gives

$$P_{n-j} A_{0}^{(n)} \leq 1 \quad \text{and} \quad \sum_{k=2}^{n} P_{n-k} A_{k-2}^{(k)} \leq \sum_{k=2}^{n} P_{n-k} A_{k-2}^{(k)} = 1.$$  

Applying the definition (3.4) with the regularity assumption, it is not difficult to get

$$G_{\text{loc}}^{1} \leq C_{v} \tau_{1}^{\sigma} / \sigma \quad \text{and} \quad G_{\text{his}}^{k} \leq C_{v} t_{k-1}^{\sigma - 3} \tau_{k}^{3} \quad \text{for} \quad 2 \leq k \leq N.$$  

Similarly, by using the formula (3.5), one gets

$$G_{\text{his}}^{1} \leq C_{v} (\tau_{1}^{\sigma} / \sigma + t_{1}^{\sigma - 3} \tau_{2}^{3}) \quad \text{and} \quad G_{\text{his}}^{k} \leq C_{v} (t_{k-1}^{\sigma - 3} \tau_{k}^{3} + t_{k}^{\sigma - 3} \tau_{k+1}^{3}) \quad \text{for} \quad 2 \leq k \leq N - 1.$$  

Then it follows from Theorem 3.4 that

$$E_{\text{glob}}^{n} \leq P_{n-1} A_{0}^{(n)} (G_{\text{loc}}^{1} + G_{\text{his}}^{1}) + \sum_{k=2}^{n} P_{n-k} A_{0}^{(k)} G_{\text{loc}}^{k} + \sum_{k=2}^{n-1} P_{n-k} A_{k-2}^{(k)} G_{\text{his}}^{k}.$$  

The first term on the right is bounded by $C_{v} (\tau_{1}^{\sigma} / \sigma + t_{1}^{\sigma - 3} \tau_{2}^{3})$, and the remaining terms can be bounded by

$$\leq \frac{C_{v}}{1 - \alpha} \max_{2 \leq k \leq n} t_{k}^{2} t_{k-1}^{\sigma - 3} \tau_{k}^{3} + \frac{C_{v}}{1 - \alpha} \max_{2 \leq k \leq n-1} \left( t_{k}^{2} t_{k-1}^{\sigma - 3} \tau_{k}^{3} + t_{k}^{\sigma + 3} \tau_{k+1}^{3} \tau_{k}^{3}\right) \leq \frac{C_{v}}{1 - \alpha} \max_{2 \leq k \leq n} t_{k}^{2} t_{k-1}^{\sigma - 3} \tau_{k}^{3} (1 + \rho_{k}^{2})$$  

implying the claimed estimate. \hfill \blacksquare
Remark 3.7. The proof of Lemma 3.6 and the ECS bound in Theorem 3.4 give

\[ |Y^{1-\theta}| \leq A_0^{(1)} G^{1}_{\text{loc}} \leq C_v \tau_1^{\sigma - \alpha} / \sigma, \]

implying that \( Y^{1-\theta} = O(1) \) when \( \sigma = \alpha \), and if \( 0 < \sigma < \alpha \) then the situation becomes worse. The global consistency analysis seems therefore to be also a superconvergence analysis.

Now we describe the contribution to the global truncation error from the time weighted terms. The next lemma suggests that the temporal error introduced by the time weighted approach is smaller than that generated by the Alikhanov approximation of the Caputo derivative.

**Lemma 3.8.** Assume that \( v \in C^2((0, T]) \), and there exists a positive constant \( C_v \) such that \( |v''(t)| \leq C_v(1 + t^{\sigma - 2}) \) for \( 0 < t \leq T \), where \( \sigma \in (0, 1) \cup (1, 2) \) is a regularity parameter. Denote the local truncation error of \( \phi^{n-\theta} \) by

\[ \mathcal{R}^{n-\theta} = v(t_{n-\theta}) - v^{n-\theta} \quad \text{for} \quad 1 \leq n \leq N. \]

If the mesh condition \( \text{M1} \) holds, then the global consistency error satisfies

\[ \sum_{j=1}^{n} P_{n-j}^{(n)} |\mathcal{R}^{j-\theta}| \leq C_v \left( \tau_1^{\sigma + \alpha} / \sigma + t_{n}^{\alpha} \max_{2 \leq k \leq n} t_{k-1}^{\sigma - 2} t_{k}^{2} \right) \quad \text{for} \quad 1 \leq n \leq N. \]

**Proof.** The following integral representation of \( \mathcal{R}^{j-\theta} \) can be easily verified, for example using the Taylor formula with integral remainder [12, Lemma 2.5],

\[ \mathcal{R}^{j-\theta} = -\theta \int_{t_{j-1}}^{t_{j}} (s - t_{j-1}) v''(s) \, ds - (1 - \theta) \int_{t_{j-\theta}}^{t_{j}} (t_{j} - s) v''(s) \, ds, \quad 1 \leq j \leq N. \]

Under the regularity assumption, one has

\[ |\mathcal{R}^{1-\theta}| \leq C_v \frac{\tau_1^{\sigma}}{\sigma} \quad \text{and} \quad |\mathcal{R}^{j-\theta}| \leq C_v t_{j-1}^{\sigma - 2} t_{j}^{2}, \quad 2 \leq j \leq N. \]

Note that Theorem 2.2 (I) implies \( A_0^{(1)} \geq \frac{4}{T} \omega_{2-\alpha}(\tau_1) / \tau_1 \), and then the identity (1.6) shows that

\[ P_{n-1}^{(n)} \leq 1 / A_0^{(1)} \leq 3 \Gamma(2 - \alpha) \tau_1^{\alpha}. \]

Therefore we obtain

\[ \sum_{j=1}^{n} P_{n-j}^{(n)} |\mathcal{R}^{j-\theta}| = P_{n-1}^{(n)} |\mathcal{R}^{1-\theta}| + \sum_{j=2}^{n} P_{n-j}^{(n)} |\mathcal{R}^{j-\theta}| \]

\[ \leq 3 \Gamma(2 - \alpha) \tau_1^{\alpha} |\mathcal{R}^{1-\theta}| + \max_{2 \leq k \leq n} |\mathcal{R}^{k-\theta}| \sum_{j=1}^{n} P_{n-j}^{(n)} \]

\[ \leq C_v \left( \tau_1^{\sigma + \alpha} / \sigma + t_{n}^{\alpha} \max_{2 \leq k \leq n} t_{k-1}^{\sigma - 2} t_{k}^{2} \right), \quad 1 \leq n \leq N, \]

where the estimate (1.8) with \( \pi_A = 11/4 \) has been used in the last inequality. \( \square \)
3.2. Convergence. We now establish the convergence of the numerical solution under the regularity conditions (1.13) and the assumptions M1–M2. To deal with the spatial error, we introduce the Ritz projector $R_h : H^1_0(\Omega) \to X_h$, defined by

$$\langle \nabla R_h v, \nabla \chi \rangle = \langle \nabla v, \nabla \chi \rangle \quad \text{for } v \in H^1_0(\Omega) \text{ and } \chi \in X_h.$$ 

Theorem 3.9. Suppose that the solution $u$ of (1.1) has the regularity property (1.13) for the parameter $\sigma \in (0,1) \cup (1,2)$, and consider the time-stepping method (1.3) using the nonuniform Alikhanov formula (1.2) with the discrete kernels (2.4). If M1 holds with the maximum step size $\tau \leq 1/\sqrt[3]{\Pi(2-\alpha)\kappa}$, then the discrete solution $u^n_h$ is convergent with respect to the $L^2$-norm,

$$\|u(t_n) - u^n_h\| \leq C_u E_\alpha(20\kappa + t_n^\alpha) \left( \frac{\tau_n^\sigma}{\sigma} + \max_{2\leq k \leq n} t_k^\alpha t_{k-1}^{\sigma-3} \frac{\tau_k^3}{\tau_{k-1}^3} + t_n^\alpha \max_{2\leq k \leq n} t_{k-1}^{\sigma-2} \right) + \|u_0 - R_h u_0\| + (t_n + t_n^\sigma + t_n^2)h^2 \quad \text{for } 1 \leq n \leq N.$$ 

In particular, if M2 also holds and if we choose $u_0 = R_h u_0$, then

$$\|u(t_n) - u^n_h\| \leq \frac{C_u}{\sigma(1-\alpha)} \tau_n^{\min(\gamma,2)} + C_u h^2 \quad \text{for } 1 \leq n \leq N,$$

where $C_u$ may depend on $u$ and $T$, but is uniformly bounded with respect to $\alpha$ and $\sigma$.

Proof. Let $e^n_h = u^n_h - R_h u^n \in X_h$ where $u^n = u(t_n)$, so that

$$\|e^n_h\| \leq \|u^n - R_h u^n\| + \|e^n_h\|.$$ 

The usual analysis of the elliptic problem shows that, under the first regularity assumption in (1.13),

$$\|u^n - R_h u^n\| \leq C_\Omega h^2 \|u^n\|_{H^2(\Omega)} \leq C_u h^2,$$

so it suffices to deal with $e^n_h$. We find [9, Section 4] that

$$\langle (D_\sigma^\alpha e^n_h - \theta, \chi) + \langle \nabla e^n_h - \theta, \nabla \chi \rangle = \kappa\langle e^n_h - \theta, \chi \rangle + \langle \mathcal{R}^n, \chi \rangle,$$

for all $\chi \in X_h$, where

$$\mathcal{R}^n = (D_\tau^\alpha u)(t_{n-\theta}) - (D_\tau^\alpha R_h u)^{n-\theta} - \kappa(u(t_{n-\theta}) - R_h u^{n-\theta}) + \Delta(u^n - \theta - u(t_{n-\theta})).$$

Choosing $\chi = u^{n-\theta}$ yields an inequality of the form (2.7) with $u^n - \theta$ and $f(t_{n-\theta})$ replaced by $e^n_h - \theta$ and $\mathcal{R}^n$, respectively. Hence, the argument leading to Theorem 2.4 shows that

$$\|e^n_h\| \leq 2E_\alpha(20\kappa + t_n^\alpha) \left( \|e^0_h\| + 2 \max_{1 \leq k \leq n} \sum_{j=1}^k P_{k-j}^{(k)} \|\mathcal{R}^j\| \right) \quad \text{for } 1 \leq n \leq N.$$ 

Write $\mathcal{R}^j = \mathcal{R}^j_1 + \mathcal{R}^j_2 + \mathcal{R}^j_3 + \mathcal{R}^j_4$, where

$$\mathcal{R}^j_1 = (D_\tau^\alpha u)(t_{j-\theta}) - (D_\tau^\alpha R_h u)^{j-\theta}, \quad \mathcal{R}^j_2 = (\kappa + \Delta)(u^{j-\theta} - u(t_{j-\theta})),$$

$$\mathcal{R}^j_3 = (D_\tau^\alpha (u - R_h u))^{j-\theta}, \quad \mathcal{R}^j_4 = \kappa(R_h u - u)^{j-\theta}.$$
Applying Lemmas 3.6 and 3.8, combined with the regularity assumption (1.13), one obtains
\[
\max_{1 \leq k \leq n} \sum_{j=1}^{k} P_{k-j}^{(k)} \| R_{j}^2 \| \leq C u \left( \frac{\tau^2}{\sigma} \min \left\{ 1, \frac{1}{\alpha} \right\} \max_{2 \leq k \leq n} t_{k-2}^{\sigma-3} \frac{\tau^3}{\tau_{k-1}} + t_{n}^{\alpha} \max_{2 \leq k \leq n} t_{k-1}^{\sigma-2} \right).
\]
Since
\[
\| R_{j}^2 \| = \left\| \sum_{\ell=1}^{j} A_{j-\ell}^{(j)} \nabla \tau (u - R_{h} u) \right\| \leq \sum_{\ell=1}^{j} A_{j-\ell}^{(j)} \int_{t_{\ell-1}}^{t_{\ell}} \| (u - R_{h} u)'(t) \| \, dt,
\]
the identity (1.6), the error bound (3.8) for the Ritz projection and the regularity assumption (1.13) give
\[
\max_{1 \leq k \leq n} \sum_{j=1}^{k} P_{k-j}^{(k)} \| R_{j}^2 \| \leq C u h^{2} \\sum_{1 \leq k \leq n} \left( \sum_{\ell=1}^{k} P_{k-j}^{(k)} A_{j-\ell}^{(j)} \right) \int_{t_{\ell-1}}^{t_{\ell}} \| (u - R_{h} u)'(t) \| \, dt
\leq C u h^{2} \int_{0}^{t_{n}} \| u'(t) \|_{H^2(\Omega)} \, dt \leq C u (t_{n} + \tau_{n}) h^{2}.
\]
Recalling the upper bound (1.8) and the Ritz projection error (3.8), we see that
\[
\max_{1 \leq k \leq n} \sum_{j=1}^{k} P_{k-j}^{(k)} \| R_{j}^2 \| \leq C u h^{2} \max_{1 \leq k \leq n} \sum_{j=1}^{k} P_{k-j}^{(k)} \| u^{\gamma} \|_{H^{2}(\Omega)} \leq C u t_{n}^{2} h^{2},
\]
so the first estimate for \( \| u_{h}^{n} - u(t_{n}) \| \) follows. If the mesh assumption M2 holds, then \( \tau_{1} \leq C_{1} \gamma \) and, with \( \beta := \min \{ 2, \gamma \sigma \}, \)
\[
(3.11) \quad t_{k}^{\sigma} t_{k-1}^{\tau_{3}} / \tau_{k-1} \leq C \gamma t_{k}^{\sigma + \tau_{3} - 3 - \alpha} \leq C \gamma t_{k}^{\sigma - 3 - \alpha} \tau_{k}^{\beta} (\tau \min \{ 1, t_{k}^{1-1/\gamma} \})^{\beta}
\leq C \gamma t_{k}^{\sigma - \beta / (\gamma + 1)} \tau_{k}^{3 - \alpha - \beta} \tau^{\beta}
\leq C \gamma t_{k}^{\max \{ 0, (3 - \alpha) / \gamma \} \tau^{\beta}}, \quad 2 \leq k \leq n.
\]
In addition, we have
\[
(3.12) \quad t_{k-1}^{\tau_{3} - 2 - \beta} \leq C \gamma t_{k}^{\tau_{3} - 2 - \beta} (\tau \min \{ 1, t_{k}^{1-1/\gamma} \})^{\beta}
\leq C \gamma t_{k}^{\tau_{3} - \beta / \gamma} (\tau_{k} / t_{k})^{\tau_{3} - \alpha - \beta} \tau^{\beta} \leq C \gamma t_{k}^{\max \{ 0, (2 - \alpha) / \gamma \} \tau^{\beta}}, \quad 2 \leq k \leq n,
\]
so the claimed second result follows immediately by noting that \( t_{n} \leq T \).

Remark 3.10. Replacing \( f(t_{n-\theta}) \) with \( f^{n-\theta} \) in (1.3) would introduce an additional term \( f^{n-\theta} - f(t_{n-\theta}) \) in the definition (3.9) of \( R_{n} \), but would not affect the final error bound, assuming \( f \) has the regularity properties needed to apply Lemma 3.8. Also, instead of \( u_{h} = R_{h} u_{0} \) we could choose the interpolant or the \( L_{2} \)-projection of \( u_{0} \) and still maintain second-order accuracy in space.

Remark 3.11. By an argument similar to that in (3.11), it is not difficult to show
\[
t_{k}^{\sigma - 3 - \alpha} \leq C \gamma t_{k}^{\max \{ 0, (3 - \alpha) / \gamma \} \tau^{\beta}},
\]
which means that the Alikhanov formula \((D_{h}^{\alpha} u)^{n-\theta}\) approximates \((D_{h}^{\alpha} u)(t_{n-\theta})\) to order \( O(\tau^{3-\alpha}) \) if \( \gamma \geq (3 - \alpha) / \sigma \). However, the term (3.12) arising from the difference \( u(t_{n-\theta}) - u_{h}^{n-\theta} \) in (3.9) would still limit the convergence rate for the overall scheme to order \( O(\tau^{2}) \).
4. Proof of Theorem 2.2 (discrete convolution kernels). Our aim is to prove the boundedness and monotonicity of the convolution kernels $A_{n-k}^{(n)}$. Since the coefficients $a_{n-k}^{(n)}$, $b_{n-k}^{(n)}$ and $A_{n-k}^{(n)}$ in (2.2), (2.3) and (2.4) are defined on nonuniform meshes, it is a technically challenging task and some new techniques will be necessary.

Note that, some techniques using Taylor expansion or function monotonicity have been applied in [1, 3, 13] to investigate the discrete convolution kernels in high-order numerical Caputo formulas. These techniques cannot be directly applied here although they would be well suited for the uniform case with $\tau_k = \tau$.

We start from the alternative definition (2.6) of $b_{n-k}^{(n)}$. Compared with the original definition (2.3), the new formula (2.6) has a nonnegative integrand because $\Gamma(-\alpha) < 0$ and $\omega_{\alpha}(t_n - \theta - s) < 0$, motivating us to consider the integrals

$$
\int_{t_{k-1}}^{t_k} \omega''_n(t) \, dt, \quad \int_{t_{k-1}}^{t_k} \frac{t - t_{k-1}}{\tau_k} \omega''_n(t) \, dt \quad \text{and} \quad \int_{t_{k-1}}^{t_k} \frac{t - t_{k-1}}{\tau_k} \omega''_n(t) \, dt.
$$

Actually, they are very close to the values of $b_{n-k}^{(n)}$ and $a_{n-k-1}^{(n)} - a_{n-k}^{(n)}$ if $\rho = O(1)$. In studying theoretical properties of the discrete kernels $A_{n-k}^{(n)}$, these integrals will play a bridging role in establishing some useful links between the underlying discrete coefficients $a_{n-k}^{(n)}$, $b_{n-k}^{(n)}$ and $A_{n-k}^{(n)}$: see Lemmas 4.2, 4.3 and 4.6.

4.1. Proof of Theorem 2.2 (I).

**Lemma 4.1.** The discrete coefficients $a_{n-k}^{(n)}$ defined in (2.2) satisfy

(i) $a_{n-k}^{(n)} > \omega_{1-\alpha}(t_n - \theta - t_{k-1}) > a_{n-k+1}^{(n)}$ for $1 \leq k \leq n$;

(ii) $a_0^{(n)} > \frac{3}{4} \int_{t_{n-1}}^{t_n} \omega_{1-\alpha}(t_n - s) \, ds$ and $a_{n-k}^{(n)} > \int_{t_{k-1}}^{t_k} \omega_{1-\alpha}(t_n - s) \, ds$ for $1 \leq k \leq n - 1$.

**Proof.** (i) If $k = n$, one has

$$
a_0^{(n)} = \frac{1 - \theta}{1 - \alpha} \omega_{1-\alpha}(t_n - t_{n-1}) > \omega_{1-\alpha}(t_n - t_{n-1}).
$$

For $1 \leq k < n$, the claimed inequalities follow directly from the integral mean value theorem and the fact that $\omega_n(s) = \omega_{1-\alpha}(t_n - s)$ is a strictly increasing function.

(ii) Also, the lower bounds of $a_{n-k}^{(n)}$ for $1 \leq k < n$ follow from the definition (2.2) immediately. For the remaining coefficient $a_0^{(n)}$, since $e^x > 1 + x$ for all real $x$ and since $\ln(1 - x/2) > -x$ for $0 < x < 1$, we find that

$$(1 - \theta)^{1-\alpha} = e^{(1-\alpha)\ln(1-\alpha/2)} > 1 + (1 - \alpha)\ln(1 - \alpha/2) > 1 - \alpha(1 - \alpha) \geq 3/4,
$$

and then $a_0^{(n)} = (1 - \theta)^{1-\alpha} \omega_{2-\alpha}(\tau_n)/\tau_n > \frac{3}{4\tau_n} \int_{t_{n-1}}^{t_n} \omega_{1-\alpha}(t_n - s) \, ds$. 

**Lemma 4.2.** The discrete coefficients $b_{n-k}^{(n)}$ defined in (2.3) satisfy

$$
0 < b_{n-k}^{(n)} \leq \frac{\rho_k}{4(1 + \rho_k)} \int_{t_{k-1}}^{t_k} \omega''_n(s) \, ds, \quad 1 \leq k \leq n - 1.
$$

**Proof.** Since $0 < (s - t_{k-1})(t_k - s) - \tau_k^2/4$ for $t_{k-1} < s < t_k$, the alternative definition (2.6) of $b_{n-k}^{(n)}$ yields the result and completes the proof.

As an application of Lemma 4.2, the next lemma builds up a link between $a_{n-k}^{(n)}$ and $b_{n-k}^{(n)}$. For a uniform mesh $t_n = n\tau$, this lemma gives

$$
0 < b_{n-k}^{(n)} < \frac{\theta}{4(n - \theta - k)} a_{n-k}^{(n)} \quad \text{for } 1 \leq k \leq n - 1.
$$
By comparison, Alikhanov [1, Lemma 3 and Corollary 2] gives \( b_{n-k}^{(n)} < \frac{\theta}{2(1-\theta)} a_{n-k}^{(n)} \).

Obviously, the new bound is much sharper.

**Lemma 4.3.** The positive coefficients \( a_{n-k}^{(n)} \), \( b_{n-k}^{(n)} \) defined in (2.2) and (2.3) satisfy

\[
b_{n-k}^{(n)} < \frac{\theta \tau_k}{2(t_n-\theta - t_k)} \frac{\rho_k}{1+\rho_k} a_{n-k}^{(n)}, \quad 1 \leq k \leq n-1.
\]

**Proof.** For fixed \( n \) and \( 1 \leq k \leq n-1 \), consider an auxiliary function

\[
\varphi_k(z) := \int_{t_{k-1}}^{t_{k-1}+z} \omega_n''(s) \, ds - \frac{2\theta}{t_n-\theta - t_k} \int_{t_{k-1}}^{t_{k-1}+z} \omega_n'(s) \, ds, \quad 0 < z < \tau_k.
\]

Since \( \omega_n''(t) = \alpha \omega_n'(t)/(t_n-\theta - t) \), the first derivative

\[
\varphi_k'(z) = \frac{\alpha - 2\theta}{t_n-\theta - t_k} = 0, \quad 0 < z < \tau_k, \quad 1 \leq k \leq n-1.
\]

Hence the definition (2.2) of \( a_{n-k}^{(n)} \) yields

\[
\int_{t_{k-1}}^{t_k} \omega_n''(s) \, ds - \frac{2\theta \tau_k}{t_n-\theta - t_k} a_{n-k}^{(n)} = \varphi_k(\tau_k) - \varphi_k(0) = 0, \quad 1 \leq k \leq n-1.
\]

Lemma 4.2 gives the claimed inequality and completes the proof. □

Now we verify Theorem 2.2 (I) by using Lemmas 4.1 and 4.3.

**Proof of Theorem 2.2 (I).** Under the assumption M1, one has \( \theta < 1-\theta, \rho_k < 7/4 \) and \( t_n-\theta - t_k \geq (1-\theta) \tau_{k+1} \) for \( 1 \leq k \leq n-1 \). Thus, by using Lemma 4.3, one has

\[
b_{n-k}^{(n)} < \frac{\theta \tau_k}{2(1-\theta) \tau_{k+1}} \frac{\rho_k}{1+\rho_k} a_{n-k}^{(n)} < \frac{7\rho_k}{8(1+\rho_k)} a_{n-k}^{(n)} < \frac{7}{11} a_{n-k}^{(n)}, \quad 1 \leq k \leq n-1,
\]

since the function \( \tau/(1+t) \) is increasing for any \( t > 0 \). By Lemma 4.1 (i), \( a_{1}^{(n)} < a_{0}^{(n)} \), then the definition (2.4) yields

\[
A_{0}^{(n)} = a_{0}^{(n)} + \rho_{n-1} b_{1}^{(n)} < a_{0}^{(n)} + \frac{4}{11} a_{0}^{(n)} = \frac{24}{11} a_{0}^{(n)}.
\]

So the definition (2.2) of \( A_{0}^{(n)} \) gives the upper bound

\[
A_{0}^{(n)} \leq \frac{24}{11 \tau_n} (1-\theta)^{1-\alpha} \int_{t_{n-1}}^{t_n} \omega_{1-\alpha}(t_n - s) \, ds \leq \frac{24}{11 \tau_n} \int_{t_{n-1}}^{t_n} \omega_{1-\alpha}(t_n - s) \, ds.
\]

The lower bounds of \( A_{n-k}^{(n)} \) for \( 1 \leq k \leq n-1 \) follow from Lemma 4.1 (ii) because the definition (2.4) implies that

\[
A_{n-k}^{(n)} \geq a_{n-k}^{(n)} - b_{n-k}^{(n)} > \frac{4}{11} a_{n-k}^{(n)}.
\]

The proof of Theorem 2.2 (I) is complete. □
4.2. Proof of Theorem 2.2 (II)–(III). For simplicity of presentation, in this subsection we let

\[(1) \quad I_{n-k}^{(n)} := \int_{t_{k-1}}^{t_k} \frac{t_k - t}{\tau_k} \varphi_n''(t) \, dt \quad \text{and} \quad J_{n-k}^{(n)} := \int_{t_{k-1}}^{t_k} \frac{t - t_{k-1}}{\tau_k} \varphi_n''(t) \, dt\]

for \(1 \leq k \leq n - 1\).

Lemma 4.4. For \(1 \leq k \leq n - 2\), the positive coefficients \(b_{n-k}^{(n)}\) in (2.3) satisfy

(i) \(I_{n-k}^{(n)} \geq \frac{1 + \rho_k}{\rho_k} b_{n-k}^{(n)}\);  \(\) (ii) \(J_{n-k}^{(n)} \geq \frac{2(1 + \rho_k)}{\rho_k} b_{n-k}^{(n)}\);  \(\) (iii) \(J_{n-k}^{(n)} \geq I_{n-k}^{(n)}\).

Proof. The alternative definition (2.6) of \(b_{n-k}^{(n)}\) gives the result (i) directly since \(0 < s - t_{k-1} < \tau_k\) for \(s \in (t_{k-1}, t_k)\). Since \(\varphi_n''(t) > 0\) for \(0 < t < t_{n-\theta}\), we take \(q := \varphi_n'\) in Lemma 2.1 to find

\[\int_{t_{k-1}}^{t_k} \left(\frac{s - t_{k-1}}{\tau_k} - \frac{1}{2}\right) \varphi_n''(s) \, ds = \frac{1}{2\tau_k} \int_{t_{k-1}}^{t_k} (s - t_{k-1})(t_k - s) \varphi_n''(s) \, ds > 0,\]

and then \(J_{n-k}^{(n)} > \frac{1}{2} t_k \int_{t_{k-1}}^{t_k} \varphi_n''(s) \, ds\) for \(1 \leq k \leq n - 1\). So the inequality (ii) follows immediately from Lemma 4.2. Moreover, \(2J_{n-k}^{(n)} > \int_{t_{k-1}}^{t_k} \varphi_n''(s) \, ds = I_{n-k}^{(n)} + J_{n-k}^{(n)}\) so the claimed result (iii) follows directly.

Lemma 4.5. For any fixed \(n\) (\(3 \leq n \leq N\)) and \(1 \leq k \leq n - 2\), it holds that

(i) \(I_{n-k}^{(n)} \geq \frac{1}{\rho_k} J_{n-k}^{(n)}\);  \(\) (ii) \(J_{n-k}^{(n)} \geq \frac{1}{\rho_k} J_{n-k}^{(n)}\).

Proof. For fixed \(n \geq 2\), introduce an auxiliary function with respect to \(z \in [0, 1]\),

\[\psi_k(z) := \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k + z\tau_k} \varphi_n''(s) \, ds, \quad 1 \leq k \leq n - 1,\]

with the first and second derivatives

\[
\psi_k'(z) = \int_{t_{k-1}}^{t_k + z\tau_k} \varphi_n''(s) \, ds, \quad \psi_k''(z) = \tau_k \varphi_n''(t_{k-1} + z\tau_k), \quad 1 \leq k \leq n - 1.
\]

Note that \(\psi_k(0) = \psi_k'(0) = 0\) for \(1 \leq k \leq n - 1\), and \(\psi_{k+1}(0) = \psi_{k+1}'(0) = 0\) for \(0 \leq k \leq n - 2\). Thanks to the Cauchy differential mean-value theorem, there exist \(z_{1k}, z_{2k} \in (0, 1)\) such that

\[\frac{J_{n-k}^{(n)}}{I_{n-k}^{(n)}} = \frac{\psi_{k+1}(1)}{\psi_k(1)} = \frac{\psi_{k+1}(1) - \psi_{k+1}(0)}{\psi_k(1) - \psi_k(0)} = \frac{\psi_k'(z_{1k})}{\psi_k'(z_{1k})} = \frac{\psi_k'(z_{1k}) - \psi_k'(z_{2k})}{\psi_k'(z_{1k}) - \psi_k'(z_{2k})} \geq \frac{1}{\rho_k}, \quad 1 \leq k \leq n - 2,
\]

because \(\varphi_n''(t) > 0\) is increasing and \(t_k > t_{k-1} + z_{2k} \tau_k\). The inequality (i) follows. We now introduce another auxiliary function for \(z \in [0, 1]\),

\[\phi_k(z) := \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k + z\tau_k} (s - t_{k-1}) \varphi_n''(s) \, ds, \quad 1 \leq k \leq n - 1,
\]

with the first derivative \(\phi_k'(z) = z\tau_k \varphi_n''(t_{k-1} + z\tau_k)\) for \(1 \leq k \leq n - 1\). Then a similar argument yields the desired result (ii) and completes the proof. \(\square\)
LEMMA 4.6. The positive coefficients $a_{n-k}^{(n)}$ in (2.2) satisfy

$$a_{n-k-1}^{(n)} - a_{n-k}^{(n)} = f_{n-k-1}^{(n)} + f_{n-k}^{(n)}, \quad 1 \leq k \leq n - 2 \ (3 \leq n \leq N),$$

and for $k = n - 1 \ (2 \leq n \leq N),$

$$a_0^{(n)} - a_1^{(n)} = \frac{\theta}{1 - 2\theta} \omega_n^t(t_{n-1}) + J_1^{(n)}.$$

Proof. For fixed $n \ (3 \leq n \leq N)$, applying the definition (2.2), we exchange the order of integration to find

$$a_{n-k-1}^{(n)} - \omega_n^t(t_k) = \int_{t_k}^{t_{k+1}} \frac{\omega_n^t(s) - \omega_n^t(t_k)}{\tau_{k+1}} \, ds = \int_{t_k}^{t_{k+1}} \int_{t_k}^{s} \frac{\omega_n^t(t)}{\tau_{k+1}} \, dt \, ds = I_{n-k-1}^{(n)}$$

for $0 \leq k \leq n - 2$, and similarly,

$$a_{n-k}^{(n)} - \omega_n^t(t_k) = \int_{t_{k-1}}^{t_k} \frac{\omega_n^t(s) - \omega_n^t(t_k)}{\tau_k} \, ds = -J_{n-k}^{(n)}$$

for $1 \leq k \leq n - 1 \ (2 \leq n \leq N)$. Hence the desired first equality is obtained by a simple subtraction. For the case of $k = n - 1 \ (2 \leq n \leq N)$, the above equality gives

$$a_1^{(n)} - \omega_n^t(t_{n-1}) = -J_1^{(n)}.$$

We have $a_0^{(n)} = \frac{1 - \theta}{1 - 2\theta} \omega_n^t(t_{n-1})$ such that $a_0^{(n)} - \omega_n^t(t_{n-1}) = \frac{\theta}{1 - 2\theta} \omega_n^t(t_{n-1})$. Thus a simple subtraction yields the second equality and completes the proof.

LEMMA 4.7. If M1 holds, the positive coefficients $a_{n-k}^{(n)}$ in (2.2) satisfy

$$a_{n-k-1}^{(n)} - a_{n-k}^{(n)} = \begin{cases} b_{n-2}^{(n)} + \frac{6}{5} f_{n-1}^{(n)}, & k = 1, \\ b_{n-k-1}^{(n)} + \rho k - 1 b_{n-k-1}^{(n)} + \frac{6}{5} f_{n-k}^{(n)}, & k > 1, \end{cases}$$

for $1 \leq k \leq n - 2 \ (3 \leq n \leq N)$, and for $k = n - 1 \ (2 \leq n \leq N),$

$$a_0^{(n)} - a_1^{(n)} \geq \begin{cases} I_1^{(2)}, & n = 2, \\ \rho n - 2 b_2^{(n)} + I_1^{(n)}, & n > 2. \end{cases}$$

Proof. For fixed $n$, applying Lemma 4.4 (i) and Lemma 4.5 (i), we obtain

$$I_{n-k-1}^{(n)} = \frac{\rho k + 1}{1 + \rho_{k+1}} I_{n-k-1}^{(n)} + \frac{I_{n-k-1}}{1 + \rho_{k+1}} \geq b_{n-k-1}^{(n)} + \frac{I_{n-k}}{\rho k (1 + \rho_{k+1})}$$

$$\geq b_{n-k-1}^{(n)} + \frac{I_{n-k}}{\rho (1 + \rho)} \geq b_{n-k}^{(n)} + \frac{16}{l t} f_{n-k}^{(n)}, \quad 1 \leq k \leq n - 2,$$

where the assumption M1 was used. By using Lemma 4.5 (ii) and Lemma 4.4 (ii),

$$\frac{\rho_{k-1}^3}{2(1 + \rho_{k-1})} f_{n-k-1}^{(n)} \geq \frac{\rho_{k-1}^2}{2(1 + \rho_{k-1})} f_{n-k}^{(n)} \geq \rho_{k-1} f_{n-k+1}^{(n)}, \quad 2 \leq k \leq n - 1.$$
Then, noting that $2 + 2x - x^3 \geq 9/64$ for $x \in [0, 7/4]$, we apply Lemma 4.4 (iii) and the assumption M1 to get

$$J_{n-k}^{(n)} = \frac{\rho_{n-1}^3}{2(1 + \rho_{n-1})} J_{n-k}^{(n)} + \frac{2 + 2\rho_{n-1} - \rho_{n-1}^3}{2(1 + \rho_{n-1})} J_{n-k}^{(n)} \geq \rho_{n-1} b_{n-k+1}^{(n)} + \frac{9}{352} J_{n-k}^{(n)},$$

where $2 \leq k \leq n - 1$. Hence, with help of (4.2)–(4.3), we apply Lemma 4.6 to find

$$a_{n-k-1}^{(n)} - a_{n-k}^{(n)} = J_{n-k-1}^{(n)} + J_{n-k}^{(n)} \geq b_{n-k-1}^{(n)} + \rho_{n-k} b_{n-k+1}^{(n)} + \left( \frac{9}{352} + \frac{16}{71} \right) J_{n-k}^{(n)}$$

$$> b_{n-k-1}^{(n)} + \rho_{n-k} b_{n-k+1}^{(n)} + \frac{1}{5} J_{n-k}^{(n)}, \quad 2 \leq k \leq n - 2.$$

If $k = 1$, by applying Lemma 4.6 with the bound (4.2) and Lemma 4.4 (iii), one has

$$a_{n-2}^{(n)} - a_{n-1}^{(n)} = I_{n-2}^{(n)} + J_{n-1}^{(n)} \geq b_{n-2}^{(n)} + \frac{16}{71} I_{n-1}^{(n)} + I_{n-1}^{(n)} \geq b_{n-2}^{(n)} + \frac{6}{5} I_{n-1}^{(n)}.$$

To complete the proof, it remains to consider the case of $k = n - 1$ ($2 \leq n \leq N$). If $n = 2$, Lemma 4.6 and Lemma 4.4 (iii) yield

$$a_0^{(2)} - a_1^{(2)} = \frac{\theta}{1 - 2\theta} \rho_1(t_1) + J_1^{(2)} > J_1^{(2)} > I_1^{(2)}.$$

Now treat the last case of $n \geq 3$. We apply Lemma 4.3 (by taking $k = n - 2$), Lemma 4.1 (i) and the given condition M1 to get

$$\rho_{n-2} b_{n-2}^{(n)} \leq \frac{\theta_0^{n-2}}{2(\tau_n - \tau_{n-2})} \frac{\rho_{n-2}^2}{1 + \rho_{n-2}} b_2^{(n)} \leq \frac{\theta_0^{n-2}}{2} \frac{\rho_{n-2}^2}{1 + \rho_{n-2}} b_2^{(n)} \leq \frac{\theta \rho_0^3}{2(1 + \rho_0)} a_0^{(n)}$$

$$= \frac{343}{352} \theta_0^{n-2} \rho_0^{n-2} \rho_{n-2}^2 b_2^{(n)} = \frac{\theta}{\tau_n} \omega_{2-\alpha}(\tau_n - \tau_{n-1}) = \frac{\theta(1 - \theta)}{1 - 2\theta} \rho_1(t_{n-1}) \leq \frac{\theta}{1 - 2\theta} \rho_1(t_{n-1}).$$

Therefore Lemma 4.6 and Lemma 4.4 (iii) lead to

$$a_0^{(n)} - a_1^{(n)} = \frac{\theta}{1 - 2\theta} \rho_1(t_{n-1}) + J_1^{(n)} > \rho_{n-2} b_{n-2}^{(n)} + I_1^{(n)}.$$

The proof is completed.

Recalling the definition (2.4), we proceed to apply Lemmas 4.6 and 4.7.

Proof of Theorem 2.2 (II). With the notation $I_{n-k}^{(n)}$ defined in (4.1), we can write the desired inequality as

$$A_{n-k-1}^{(n)} - A_{n-k}^{(n)} \geq (1 + \rho_k) b_{n-k}^{(n)} + \frac{1}{5} J_{n-k}^{(n)}, \quad 1 \leq k \leq n - 1,$$

and treat four separate cases covering all possibilities. Indeed, from the definition (2.4) of $A_{n-k}^{(n)}$, it is not difficult to verify that

1. If $k = 1$ for $n = 2$,

$$A_0^{(2)} - A_1^{(2)} = (1 + \rho_1) b_1^{(2)} + a_0^{(2)} - a_1^{(2)}.$$

2. If $k = n - 1$ for $n \geq 3$,

$$A_0^{(n)} - A_1^{(n)} = (1 + \rho_{n-1}) b_1^{(n)} + a_0^{(2)} - a_1^{(2)} - \rho_{n-2} b_2^{(n)}.$$
Lemma 4.7

2.2 directly and completes the proof. Theorem 3.9 shows that

Theorem 3.9, we expect the temporal error dominates when \( N \leq 2,048 \). Thus, from Theorem 3.9, we expect the \( L_{\infty}(L_2) \)-error \( e(N) := \max_{1 \leq n \leq N} \| u_h^n - u(t_n) \| \) to behave like \( O(\tau^{\min(\gamma, \sigma)}) \).

We tested the sharpness of this prediction by four scenarios:
Table 5.1: Numerical temporal accuracy for $\sigma = 1 + \alpha$ and $\gamma = 1$. 

| $N$  | $\alpha = 0.4, \sigma = 1.4$ | $\alpha = 0.6, \sigma = 1.6$ | $\alpha = 0.8, \sigma = 1.8$ |
|------|-----------------|-----------------|-----------------|
|      | $e(N)$ Order    | $e(N)$ Order    | $e(N)$ Order    |
| 64   | 2.78e-04        | 2.32e-04        | 1.62e-04        |
| 128  | 7.24e-05 1.94  | 5.97e-05 1.96  | 4.13e-05 1.97  |
| 256  | 1.87e-05 1.95  | 1.52e-05 1.97  | 1.05e-05 1.97  |
| 512  | 4.74e-06 1.97  | 3.85e-06 1.98  | 2.68e-06 1.98  |
| 1024 | 1.59e-06 1.58  | 9.72e-07 1.99  | 6.80e-07 1.98  |
| 2048 | 5.61e-07 1.50  | 2.45e-07 1.99  | 1.73e-07 1.97  |
| 4096 | 2.01e-07 1.48  | 6.06e-08 2.02  | 4.52e-08 1.94  |
| 8192 | 5.83e-08 1.46  | 1.23e-08 1.98  | 1.01e-08 1.83  |

$\min\{\gamma \sigma, 2\}$ 1.40 1.60 1.80

Table 5.2: Numerical temporal accuracy for $\sigma = 1.2$ and $\alpha = 0.4$. 

| $N$  | $\gamma = 1$ | $\gamma = 5/3 = \gamma_{opt}$ | $\gamma = 2$ |
|------|--------------|-------------------------------|--------------|
|      | $e(N)$ Order | $e(N)$ Order                  | $e(N)$ Order |
| 64   | 2.98e-04     | 1.29e-04                      | 2.12e-04     |
| 128  | 8.52e-05 1.81| 3.08e-05 2.07                 | 5.07e-05 2.07|
| 256  | 2.97e-05 1.52| 7.38e-06 2.06                 | 1.24e-05 2.03|
| 512  | 1.18e-06 1.33| 1.77e-06 2.05                 | 3.02e-06 2.04|
| 1024 | 4.81e-06 1.30| 4.21e-07 2.07                 | 7.22e-07 2.06|
| 2048 | 1.98e-06 1.27| 9.25e-08 2.19                 | 1.65e-07 2.12|

$\min\{\gamma \sigma, 2\}$ 1.20 2.00 2.00

Table 5.3: Numerical temporal accuracy for $\sigma = 0.8$ and $\alpha = 0.4$. 

| $N$  | $\gamma = 2$ | $\gamma = 5/2 = \gamma_{opt}$ | $\gamma = 3$ |
|------|--------------|-------------------------------|--------------|
|      | $e(N)$ Order | $e(N)$ Order                  | $e(N)$ Order |
| 64   | 3.52e-04     | 5.28e-04                      | 5.04e-04     |
| 128  | 8.17e-05 2.11| 1.22e-04 2.11                 | 1.17e-04 2.09|
| 256  | 1.93e-05 2.08| 2.93e-05 2.07                 | 2.83e-05 2.06|
| 512  | 4.54e-06 2.08| 7.02e-06 2.06                 | 6.86e-06 2.05|
| 1024 | 1.08e-06 2.07| 1.69e-06 2.05                 | 1.68e-06 2.02|
| 2048 | 3.27e-07 1.73| 4.29e-07 1.98                 | 4.28e-07 1.97|

$\min\{\gamma \sigma, 2\}$ 1.60 2.00 2.00

*Table 5.1: $\sigma = 1 + \alpha$ and $\gamma = 1$ with fractional orders $\alpha = 0.4, 0.6$ and 0.8.*  
*Table 5.2: $\sigma = 1.2$ and $\alpha = 0.4$ with mesh parameters $\gamma = 1, 5/3$ and 2.*  
*Table 5.3: $\sigma = 0.8$ and $\alpha = 0.4$ with mesh parameters $\gamma = 2, 5/2$ and 3.*  
*Table 5.4: $\sigma = 0.4$ and $\alpha = 0.4$ with mesh parameters $\gamma = 2, 5/2$ and 5.*  

The empirical order of convergence, listed as “Order” in the tables, was computed in the usual way by supposing that $e(N) \approx C_u \tau^q$ and evaluating the convergence rate $q \approx \log_2\{e(N)/e(2N)\}$. The optimal mesh parameter $\gamma_{opt} := 2/\sigma$ is the smallest value...
Table 5.4
Numerical temporal accuracy for $\sigma = 0.4$ and $\alpha = 0.4$.

| $N$ | $\gamma = 2$ | $\gamma = 5/2$ | $\gamma = 5 = \gamma_{\text{opt}}$ |
|-----|--------------|----------------|--------------------------------|
|     | $e(N)$ Order | $e(N)$ Order   | $e(N)$ Order                   |
| 64  | 8.30e-03 -   | 4.61e-03 -     | 2.04e-03 -                     |
| 128 | 4.53e-03 0.87| 2.23e-03 1.00  | 4.82e-04 2.08                 |
| 256 | 2.56e-03 0.83| 1.11e-03 1.01  | 1.22e-04 2.11                 |
| 512 | 1.45e-03 0.82| 5.51e-04 1.00  | 2.66e-05 2.08                 |
| 1024| 8.25e-04 0.81| 2.74e-04 1.01  | 6.40e-06 2.05                 |
| 2048| 4.71e-04 0.81| 1.37e-04 1.00  | 1.58e-06 2.02                 |
| min{$\gamma \sigma, 2$} | 0.80          | 1.00           | 2.00                          |

of $\gamma$ for which we expect second-order convergence; for $\gamma > \gamma_{\text{opt}}$ we still expect second-order convergence but with a constant factor that grows with $\gamma$. The convergence behaviour is always as expected, but it is interesting to observe that, for larger values of $\sigma$ (corresponding to a less singular solution), the order can be close to 2 on the coarser grids. In such cases, the predicted convergence order is not observed until the total number $N$ of time levels is quite large.

6. Concluding remarks. An ECS analysis, including a reasonable ECS hypothesis and a global consistency error, is proposed for investigating a class of numerical approximations to the Caputo fractional derivative, employing piecewise polynomial interpolation on general nonuniform time meshes. The global consistency error bound (1.9) reveals an interesting behavior: the global approximate error of numerical Caputo formula would be “local” despite being naturally nonlocal, by choosing the time mesh according to the error equidistribution principle. The effectiveness of the ECS analysis is shown for the familiar L1 formula in [8, 11], and for the higher-order Alikhanov formula in this paper. In the latter case, the theoretical properties of the discrete convolution kernels (Theorem 2.2) and a new interpolation error formula with integral remainder for quadratic polynomials (Lemma 3.3) are crucial to obtaining a useful ECS bound of the local truncation error.

As our answer to the problem formulated in section 1, the fractional Crank–Nicolson time-stepping scheme (1.3) for the linear reaction-subdiffusion equation (1.1) is stable (Theorem 2.4) and convergent (Theorem 3.9) on general nonuniform grids satisfying a mild restriction ($\rho = 7/4$) on the local time step-size ratio. Consequently, some adaptive step-size control with $\tau_{\text{next}}/\tau_{\text{current}} \geq 4/7$ is permitted to resolve certain complex behaviors of the solution arising in nonlinear time-fractional PDEs, but a sudden, drastic reduction of the step size should be avoided to ensure stability. For the linear case, a sharp $L^2$-norm error estimate of the numerical solution is also presented (Theorem 3.9), demonstrating that a graded mesh can effectively resolve the initial singularity.

The present results lead naturally to another question: can an ECS analysis be applied to other high-order numerical Caputo formulas such as the BDF2-like (L1-2) approximation [3, 9, 10, 13]? We plan to address this issue in further research.

Acknowledgements. Hong-lin Liao thanks Prof. Ying Zhao for her valuable discussions and fruitful suggestions, and the hospitality of Beijing Computational
Science Research Center during the period of his visit.

**Appendix A. Proof of Lemma 3.3.**

For fixed $n$ and $1 \leq k \leq n - 1$, let $\ell_{k,j}(t)$ ($j = k - 1, k, k+1$) be the basis functions of quadratic Lagrange interpolation $\Pi_{2,k}v$ at the points $t_{k-1}$, $t_k$ and $t_{k+1}$. Firstly, we will express the interpolation error $(\Pi_{2,k}v)(t) = v(t) - (\Pi_{2,k}v)(t)$ in an integral form. To do so, recall two basic properties of basis functions, $\ell_{k,j}(t) = \delta_{j\nu}$ and

$$A.1 \quad \sum_{j=k-1}^{k+1} \ell_{k,j}(t)(t_j - t)^\nu = \delta_{0\nu}, \quad \nu \in \{0, 1, 2\},$$

where $\delta_{j\nu}$ and $\delta_{0\nu}$ are Kronecker delta functions. Now applying the Taylor’s expansion with integral remainder, one has

$$v(t_j) = \sum_{m=0}^{2} \frac{v^{(m)}(t)}{m!}(t_j - t)^m + \frac{1}{2} \int_{t_j}^{t_k} (t_j - s)^2 v'''(s) \, ds, \quad j \in \{k - 1, k, k+1\}.$$

Since $(\Pi_{2,k}v)(t) = \sum_{j=k-1}^{k+1} \ell_{k,j}(t)v(t_j)$, a simple combination with the three weights (basis functions) $\ell_{k,j}(t)$ ($j = k - 1, k, k+1$) gives the interpolation error

$$A.2 \quad (\widetilde{\Pi}_{2,k}v)(t) = \frac{1}{2} \sum_{j=k-1}^{k+1} \int_{t_j}^{t} \ell_{k,j}(t)(t_j - s)^2 v'''(s) \, ds, \quad t_{k-1} \leq t \leq t_{k+1},$$

because the property (A.1) implies that

$$\sum_{j=k-1}^{k+1} \ell_{k,j}(t) \sum_{m=0}^{2} \frac{v^{(m)}(t)}{m!}(t_j - t)^m = \sum_{m=0}^{2} \frac{v^{(m)}(t)}{m!} \sum_{j=k-1}^{k+1} \ell_{k,j}(t)(t_j - t)^m = v(t).$$

Furthermore, differentiating both sides of (A.2), one applies (A.1) again to get

$$A.3 \quad (\widetilde{\Pi}_{2,k}v)'(t) = \frac{1}{2} v'''(t) \sum_{j=k-1}^{k+1} \ell_{k,j}(t)(t_j - t)^2 + \frac{1}{2} \int_{t_j}^{t} \ell_{k,j}'(t)(t_j - s)^2 v'''(s) \, ds = \sum_{j=k-1}^{k+1} L_j(v)$$

for $t_{k-1} \leq t \leq t_{k+1}$, where

$$L_j(v) := \frac{1}{2} \int_{t_j}^{t} \ell_{k,j}'(t)(t_j - s)^2 v'''(s) \, ds, \quad j \in \{k - 1, k, k+1\}.$$

Secondly, we express the required integration error $\int_{t_{k-1}}^{t_k} q'(t)(\widetilde{\Pi}_{2,k}v)'(t) \, dt$ in terms of $\Pi_{1,k}q$ by using (A.3). Since

$$\ell_{k,k+1}'(t) = \frac{2}{(\tau_{k+1} + \tau_k)\tau_{k+1}} (t - t_{k-1}/2),$$

**Lemma 2.1** yields

$$\int_{t_{k-1}}^{t_k} \ell_{k,k+1}'(t)q'(t) \, dt = 2 \int_{t_{k-1}}^{t_k} \frac{(t - t_{k-1}/2)q'(t) \, dt}{(\tau_{k+1} + \tau_k)\tau_{k+1}} = -2 \int_{t_{k-1}}^{t_k} \frac{(\Pi_{1,k}q)(t) \, dt}{(\tau_{k+1} + \tau_k)\tau_{k+1}}.$$
Thus applying the formula for $L_{k+1}(v)$, we exchange the order of integration to find

\[(A.4)\quad \int_{t_k}^{t_k} q'(t)L_k(v)\,dt = \frac{1}{2} \int_{t_k}^{t_k} \ell'_{k,k+1}(t)q'(t)\,dt \int_{t_k}^{t_k} (t_k + s)^2 v''(s)\,ds\]

\[
= \frac{1}{2} \int_{t_k}^{t_k} \ell'_{k,k+1}(t)q'(t)\,dt \int_{t_k}^{t_k} (t_k + s)^2 v''(s)\,ds \\
- \frac{1}{2} \int_{t_k}^{t_k} \ell'_{k,k+1}(t)q'(t)\,dt \int_{t_k}^{t_k} (t_k - s)^2 v''(s)\,ds \\
= \int_{t_k}^{t_k} (t_k - s)^2 v''(s)\,ds \int_{t_k}^{t_k} \frac{(\overline{\Pi_{1,k}}q)(t)}{\tau_k + \tau_k} dt \\
- \frac{1}{2} \int_{t_k}^{t_k} \left[ (t_k - s)^2 v''(s) \right] \ell'_{k,k+1}(t)q'(t)\,dt \,v''(s)\,ds.
\]

Similarly, it is easy to check the following equality

\[
\ell'_{k,k-1}(t) = \frac{2t - t_k - t_{k+1}}{\tau_k} = \frac{2}{\tau_k + \tau_k} (t - t_{k-1}/2) - \frac{1}{\tau_k},
\]

and it follows that

\[
\int_{t_k}^{t_k} \ell'_{k,k-1}(t)q'(t)\,dt = 2 \int_{t_k}^{t_k} \frac{(t - t_{k-1}/2)}{\tau_k} q'(t)\,dt - 1 \int_{t_k}^{t_k} q'(t)\,dt \\
= -2 \int_{t_k}^{t_k} \frac{(\overline{\Pi_{1,k}}q)(t)}{\tau_k + \tau_k} dt - \frac{1}{\tau_k} \int_{t_k}^{t_k} q'(t)\,dt.
\]

So applying the formula of $L_{k-1}(v)$, we exchange the order of integration to find

\[(A.5)\quad \int_{t_k}^{t_k} q'(t)L_{k-1}(v)\,dt = \frac{1}{2} \int_{t_k}^{t_k} q'(t) \int_{t_k}^{t_k} \ell'_{k,k-1}(t)(t_k - s)^2 v''(s)\,ds\,dt \\
= \frac{1}{2} \int_{t_k}^{t_k} (t_k - s)^2 v''(s)\,ds \int_{t_k}^{t_k} \ell'_{k,k-1}(t)q'(t)\,dt \\
= \frac{1}{2} \int_{t_k}^{t_k} (t_k - s)^2 v''(s)\,ds \int_{t_k}^{t_k} \ell'_{k,k-1}(t)q'(t)\,dt \\
- \frac{1}{2} \int_{t_k}^{t_k} (t_k - s)^2 v''(s)\,ds \int_{t_k}^{t_k} \ell'_{k,k-1}(t)q'(t)\,dt \\
= -\int_{t_k}^{t_k} (t_k - s)^2 v''(s)\,ds + \int_{t_k}^{t_k} \frac{(\overline{\Pi_{1,k}}q)(t)}{\tau_k + \tau_k} dt \\
- \frac{1}{2} \int_{t_k}^{t_k} \left[ \int_{t_k}^{t_k} \frac{q'(t)}{\tau_k} dt + \int_{t_k}^{t_k} \ell'_{k,k-1}(t)q'(t)\,dt \right] (t_k - s)^2 v''(s)\,ds.
\]

For the remaining term involving $L_k(v)$, one has

\[
\int_{t_k}^{t_k} q'(t)L_k(v)\,dt = \frac{1}{2} \int_{t_k}^{t_k} q'(t) \int_{t_k}^{t_k} \ell'_{k,k}(t)(t_k - s)^2 v''(s)\,ds\,dt \\
= -\frac{1}{2} \int_{t_k}^{t_k} \left[ (t_k - s)^2 \int_{t_k}^{t_k} \ell'_{k,k}(t)q'(t)\,dt \right] v''(s)\,ds.
\]
Then collecting the three equalities (A.4)–(A.6), one applies the formula (A.3) to get

\[
\int_{t_k-1}^{t_k} q'(s) (\Pi_{2,k})'(s) \, ds = \int_{t_k}^{t_{k+1}} (t_{k+1} - s)^2 v''(s) \, ds \int_{t_k-1}^{t_k} \frac{(\Pi_{1,k}q)(t) \, dt}{(\tau_{k+1} + \tau_k)\tau_{k+1}} \\
- \int_{t_k-1}^{t_k} (s - t_{k-1})^2 v''(s) \, ds \int_{t_k-1}^{t_k} \frac{(\Pi_{1,k}q)(t) \, dt}{(\tau_{k+1} + \tau_k)\tau_k} + \int_{t_k-1}^{t_k} K_q(s)v'''(s) \, ds,
\]

where the integral kernel

\[
\text{(A.7)} \quad K_q(s) := -\frac{(t_{k-1} - s)^2}{2\tau_k} \int_{t_{k-1}}^{t_k} q'(t) \, dt - \frac{1}{2} \sum_{j=k-1}^{k+1} (t_j - s)^2 \int_{t_{k-1}}^{t_k} \ell'_{k,j}(t)q'(t) \, dt.
\]

Finally, to complete the proof, it remains to verify

\[
\text{(A.8)} \quad K_q(s) = \int_{t_{k-1}}^{s} (\Pi_{1,k}q)(t) \, dt, \quad t_{k-1} \leq s \leq t_k.
\]

Differentiating the identity \((t - s)^2 = \sum_{j=k-1}^{k+1} (t_j - s)^2 \ell_{k,j}(t)\), we have

\[
\sum_{j=k-1}^{k+1} (t_j - s)^2 \ell'_{k,j}(t) = 2(t - s), \quad t_{k-1} \leq s \leq t_{k+1}.
\]

Thus it follows from (A.7) that

\[
K_q(s) = -\frac{(t_{k-1} - s)^2}{2\tau_k} \int_{t_{k-1}}^{t_k} q'(t) \, dt - \int_{t_{k-1}}^{s} (t - s)q'(t) \, dt.
\]

We see that \(K_q(t_{k-1}) = 0\) and

\[
K'_q(s) = q(s) - q(t_{k-1}) - \frac{q(t_k) - q(t_{k-1})}{\tau_k} (s - t_{k-1}) = (\Pi_{1,k}q)(s), \quad t_{k-1} \leq s \leq t_k,
\]

which leads to the desired result (A.8) immediately since \(K_q(s) = \int_{t_{k-1}}^{s} K'_q(t) \, dt\).

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