

AN L_1 APPROXIMATION FOR A FRACTIONAL REACTION-DIFFUSION EQUATION, A SECOND-ORDER ERROR ANALYSIS OVER TIME-GRADED MESHES*

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Abstract. A time-stepping L_1 scheme for subdiffusion equation with a Riemann–Liouville time-fractional derivative is developed and analyzed. This is the first paper to show that the L_1 scheme for the model problem under consideration is second-order accurate (sharp error estimate) over nonuniform time-steps. The established convergence analysis is novel, innovative and concise. For completeness, the L_1 scheme is combined with the standard Galerkin finite elements for the spatial discretization, which will then define a fully-discrete numerical scheme. The error analysis for this scheme is also investigated. To support our theoretical contributions, some numerical tests are provided at the end. The considered (typical) numerical example suggests that the imposed time-graded meshes assumption can be further relaxed.

Key words. Fractional diffusion, L_1 approximations, finite element method, optimal error analysis, graded meshes

1. Introduction. Consider the following time-fractional diffusion equation,

$$(1) \quad \partial_t u(x, t) + \partial_t^{1-\alpha} \mathcal{A}u(x, t) = f(x, t), \quad \text{for } x \in \Omega \text{ and } 0 < t < T,$$

with initial condition $u(x, 0) = u_0(x)$, where $\partial_t = \partial/\partial t$, Ω is a convex polyhedral domain in \mathbb{R}^d ($d \geq 1$), and the spatial elliptic operator

$$\mathcal{A}u(x, t) = -\nabla \cdot (\kappa_\alpha(x) \nabla u(x, t)) + d(x)u(x, t).$$

The diffusivity coefficient $c_1 \leq \kappa_\alpha \leq c_2$ on Ω for some positive constants c_1 and c_2 , and the reaction coefficient d is such that the bilinear form associated with the elliptic operator \mathcal{A} (see (5)) is positive definite on the Sobolev space $H_0^1(\Omega)$. That is, it is sufficient (but not necessary) to impose that $d \geq 0$ on Ω . Both, κ and d are assumed to be sufficiently regular functions.

The fractional exponent is restricted to the range $0 < \alpha < 1$ and the fractional derivative is taken in the Riemann–Liouville sense, that is, $\partial_t^{1-\alpha} u = \partial_t \mathcal{I}^\alpha u$, where the fractional integration operator \mathcal{I}^α is defined by

$$\mathcal{I}^\alpha v(t) = \int_0^t \omega_\alpha(t-s)v(s) ds, \quad \omega_\alpha(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)}.$$

We impose a homogeneous Dirichlet boundary condition,

$$(2) \quad u(x, t) = 0 \quad \text{for } x \in \partial\Omega \text{ and } 0 < t < T.$$

Over the last decade, various time-stepping numerical methods were investigated for solving the fractional diffusion equation (1), see for example [24, 26] and related references therein. The motivation of this paper is propose and analyze a second-order accurate time-stepping L_1 scheme for solving the model problem (1). A nonuniform time mesh is employed (see (6)) to compensate for the singularity of the continuous solution near $t = 0$ [18, 22]. Such graded meshes (6) were originally used in the

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context of Volterra integral equations with weakly singular kernels, see for example [2, 3, 4], and see also [25] for a recent concrete superconvergence error analysis. Later on, time-graded meshes were successfully used to improve the performance of different numerical methods applied to fractional diffusion and fractional wave equations, see for instance [19, 23, 24, 27]. Nonuniform meshes are flexible and reasonably convenient for practical implementation, however they can significantly complicate the numerical error analysis of schemes. The time-graded mesh properties are carefully used in our error analysis to achieve optimal-order convergence rates. The designed approach is novel and concise, some innovative ideas are employed to estimate efficiently certain candidates. For completeness, we discretize in space using the standard Galerkin finite elements, where the error analysis is also examined.

To the best of our knowledge, we are not aware of any work that showed a second-order error bounds of the popular time-stepping $L1$ scheme applied to the model problem (1). However, for the time-fractional (Caputo derivative) diffusion problem (often assuming κ to be constant and the reaction coefficient d to be zero):

$$(3) \quad \mathcal{I}^{1-\alpha} \partial_t u(x, t) + \mathcal{A}u(x, t) = f(x, t), \quad \text{for } x \in \Omega \text{ and } 0 < t < T,$$

various types of $L1$ time-stepping schemes were developed and studied over the last decade, see for example [1, 5, 8, 9, 10, 15, 16, 17, 30, 32, 33, 34, 35]. In most studies, a convergence rate of order $2 - \alpha$ was proved. Furthermore, the singularity of the continuous solution u near $t = 0$ was taken into account in a few papers only, however the rest frequently ignored this fact. In contrast, a time-stepping discontinuous Petrov-Galerkin method using piecewise polynomials of degree m was introduced and analyzed in [27] for solving problem (3). For the special case $m = 1$, this method reduces to a second-order accurate time-stepping $L1$ scheme as the numerical results suggested therein, see [27, Section 5].

Outline of the paper. In section 2, we define our semi-discrete time-stepping $L1$ approximation scheme (see (9)) and describe briefly the implementation steps. Section 3 is dedicated to show our sharp error results. It is assumed that the continuous solution u of problem (1) satisfies the following regularity properties:

$$(4) \quad \|u(t)\|_2 \leq M \quad \text{and} \quad \|u'(t)\|_2 + t^{1-\alpha/2} \|u''(t)\|_1 + t^{2-\alpha/2} \|u'''(t)\|_1 \leq Mt^{\sigma-1},$$

for some positive constants M and σ . In (4), $'$ denotes the time partial derivative and $\|\cdot\|_\ell$ is the norm on the usual Sobolev space $H^\ell(\Omega)$ which reduces to the $L_2(\Omega)$ -norm when $\ell = 0$ denoted by $\|\cdot\|$. As an example, when $f(t) \equiv 0$ and $u_0 \in H_0^1(\Omega) \cap H^{2.5^-}(\Omega)$, these assumptions hold true for $\sigma = \frac{\alpha^-}{4}$, see [18, 22] for more details.

At each time level t_n , an optimal $O(\tau^2 t_n^{\sigma+\alpha-2/\gamma})$ -rate of convergence is proved in Theorem 3.5, assuming that the time mesh exponent $\gamma > \max\{2/(\sigma + \alpha/2), 2/(\sigma + 3\alpha/2 - 1/2)\}$ (see (6) for the definition of the time-graded mesh). Noting that, for $1/2 \leq \alpha < 1$ (which is practically the interesting case in terms of subdiffusion), $\sigma + \alpha/2 \leq \sigma + 3\alpha/2 - 1/2$, and so it is sufficient to assume $\gamma > 2/(\sigma + \alpha/2)$. Our error analysis involves various types of clever splitting of the error terms followed by a careful estimation of each one of them. We avoid using any versions of the weakly singular discrete Gronwall's inequalities [7, Theorem 6.1] to guarantee that the error coefficients do not blowup exponentially with the time level t_n . At the preliminary stage, our error analysis makes use of the inequality in the next lemma [21, Lemma 2.3] which will eventually enable us to establish pointwise estimates for certain terms.

LEMMA 1.1. *Let $0 < \alpha \leq 1$. If the function ϕ is in the space $W_1^1((0, t); L_2(\Omega))$ satisfies $\phi(0) = \mathcal{I}^\alpha \phi'(0) = 0$, then*

$$\|\phi(t)\|^2 \leq 2\omega_{2-\alpha}(t) \int_0^t \langle \mathcal{I}^\alpha \phi'(t), \phi'(t) \rangle dt,$$

where $\langle u, v \rangle$ is the L_2 -inner product on the spatial domain Ω .

Although the main scope of this paper is on the optimal error analysis of the time-stepping $L1$ scheme, the error analysis from the full discretization is also studied. In section 4, the semi-discrete time-stepping scheme (9) is discretized in space via the standard continuous piecewise-linear Galerkin method (see (28)), which will then define a fully-discrete numerical method. The implementation of the fully-discrete solution is briefly discussed. Compared to the error analysis in section 3, an additional term has occurred. Consequently, an additional error of order $O(h^2)$ (h is the maximum spatial mesh element size) is derived assuming that $\sigma > (1 - \alpha)/2$, see Theorem 4.1. Numerically, it is observed that this condition is not necessary. In this part of our error analysis, the next lemma [28, Lemma 3.1] is used.

LEMMA 1.2. *If the functions ϕ and ψ are in the space $L_2((0, t); L_2(\Omega))$, then for $0 < \alpha < 1$ and for $\epsilon > 0$,*

$$\left| \int_0^t \langle \phi, \mathcal{I}^\alpha \psi \rangle ds \right| \leq \frac{1}{4\epsilon(1-\alpha)^2} \int_0^t \langle \phi, \mathcal{I}^\alpha \phi \rangle ds + \epsilon \int_0^t \langle \psi, \mathcal{I}^\alpha \psi \rangle ds.$$

Unfortunately, the coefficient $\frac{1}{(1-\alpha)^2}$ blows up as α approaches 1^- , and consequently, the error bounds blowup. Such a blowup phenomenon, which was highlighted and investigated recently in [6], occurs in the error analysis (but not in numerical experiments [20]) of various numerical methods applied to different time-fractional diffusion models, see for example [11, 12, 13, 14, 15, 20, 26, 27, 30]. This blowup behavior appears to be an artifact of the method of proof, see Remark 4.2 where the blowup coefficient is controlled assuming that $\sigma > (1 - \alpha)/2$. To validate this, some compatibility conditions on the initial data u_0 (for example, $u_0 \in H^{2+1/\alpha}(\Omega)$ with $u_0, \mathcal{A}u_0 \in H_0^1(\Omega)$) and also on the source term f are needed. Noting that, in the limiting case, $\alpha \rightarrow 1^-$, problem (1) reduces to the classical equation (10) and our fully-discrete scheme in (28) amounts to the standard time-stepping Crank-Nicolson (see (11)) combined with the (linear) spatial standard continuous Galerkin method. A straightforward analysis leads to an optimal time-space second-order convergence rate [31].

Finally, in section 5, a second-order convergence of the $L1$ scheme is confirmed numerically on a typical sample of test problem. When the time error is dominant, the numerical numbers in Tables 1–3 illustrate $O(\tau^{\min\{\gamma(\sigma+\alpha), 2\}})$ -rates for different choices of the time-graded mesh exponent γ and the fractional exponent α . These results indicate that the condition $\gamma > \max\{2/(\sigma + \alpha/2), 2/(\sigma + 3\alpha/2 - 1/2)\}$ in Theorem 3.5 is pessimistic. Practically, it is enough to choose $\gamma = 2/(\sigma + \alpha)$ to guarantee an $O(\tau^2)$ accuracy. Furthermore, the numerical results in Table 4 showed $O(h^2)$ -rates of convergence in space for different values of α even though the assumption $\sigma > (1 - \alpha)/2$ is not satisfied.

For later use, $A(\cdot, \cdot) : H_0^1(\Omega) \times H_0^1(\Omega) \rightarrow \mathbb{R}$ denotes the bilinear form associated with the elliptic operator \mathcal{A} , which is symmetric and positive definite, defined by

$$(5) \quad A(v, w) = \langle \kappa_\alpha \nabla v, \nabla w \rangle + \langle d v, w \rangle.$$

Throughout the paper, C is a generic constant which may depend on the parameters M, σ, T, Ω , and γ , but is independent of τ and h .

2. Numerical method. This section is devoted to introduce our semi-discrete time-stepping $L1$ numerical scheme for solving the model problem (1). We use a time-graded mesh with the following nodes:

$$(6) \quad t_i = (i\tau)^\gamma, \quad \text{for } 0 \leq i \leq N, \quad \text{for } \gamma \geq 1, \quad \text{with } \tau = T^{1/\gamma}/N,$$

where N is the number of subintervals. Denote by $\tau_n = t_n - t_{n-1}$ the length of the n th subinterval $I_n = (t_{n-1}, t_n)$, for $1 \leq n \leq N$. It is not hard to show that such a time-graded mesh has the following properties [19]: for $n \geq 2$,

$$(7) \quad t_n \leq 2^\gamma t_{n-1}, \quad \gamma \tau t_{n-1}^{1-1/\gamma} \leq \tau_n \leq \gamma \tau t_n^{1-1/\gamma}, \quad \tau_n - \tau_{n-1} \leq C_\gamma \tau^2 \min(1, t_n^{1-2/\gamma}).$$

For a given function v defined on the time interval $[0, T]$, let $v^n = v(t_n)$ for $0 \leq n \leq N$. With this grid function, we associate the backward difference,

$$\partial v^n = \frac{v^n - v^{n-1}}{\tau_n}.$$

To define our time-stepping numerical scheme, integrating problem (1) over the time interval I_n ,

$$(8) \quad \int_{t_{n-1}}^{t_n} u'(t) dt + \int_{t_{n-1}}^{t_n} \partial_t^{1-\alpha} \mathcal{A}u(t) dt = \int_{t_{n-1}}^{t_n} f(t) dt.$$

Our $L1$ approximate solution U , which is a continuous linear polynomial in the time variable on each closed subinterval $[t_{n-1}, t_n]$, is defined by replacing u with U in (8),

$$(9) \quad U^n - U^{n-1} + \int_{t_{n-1}}^{t_n} \partial_t^{1-\alpha} \mathcal{A}U(t) dt = \int_{t_{n-1}}^{t_n} f(t) dt, \quad \text{for } 1 \leq n \leq N,$$

with $U^0 = u_0$. As $\alpha \rightarrow 1^-$, the fractional model problem (1) amounts to the classical reaction-diffusion equation:

$$(10) \quad u'(x, t) + \mathcal{A}u(x, t) = f(x, t), \quad \text{for } x \in \Omega \text{ and } 0 < t < T,$$

and the time-stepping $L1$ numerical scheme (9) reduces to

$$(11) \quad U^n - U^{n-1} + \tau_n \mathcal{A}(U^n + U^{n-1})/2 = \int_{t_{n-1}}^{t_n} f(t) dt,$$

which is the time-stepping Crank-Nicolson method for problem (10). Motivated by this, a generalized Crank-Nicolson scheme for the fractional reaction-diffusion equation (1), defined by

$$(12) \quad U^n - U^{n-1} + \int_{t_{n-1}}^{t_n} \partial_t^{1-\alpha} \mathcal{A}\bar{U}(t) dt = \int_{t_{n-1}}^{t_n} f(t) dt, \quad \text{with } U^0 = u_0,$$

was developed in [24], where $\bar{U}(t) = (U^j + U^{j-1})/2$ for $t \in I_j$. Therein, the theoretical and numerical convergence results confirmed $O(\tau^{1+\alpha})$ -rates in time over sufficiently time-graded meshes. Both schemes (9) and (12) are computationally similar, however the theoretical and numerical results show better convergence rates of the $L1$ scheme.

For computational purposes, putting

$$\omega_{nj} = \int_{t_{j-1}}^{t_j} \omega_\alpha(t_n - s) ds \quad \text{and} \quad \widehat{\omega}_{nj} = \int_{t_{j-1}}^{t_j} \int_s^{t_j} \omega_\alpha(t_n - q) dq ds, \quad \text{for } j \leq n.$$

Hence

$$\int_{t_{n-1}}^{t_n} \partial_t^{1-\alpha} U(t) dt = (\mathcal{I}^\alpha U)(t_n) - (\mathcal{I}^\alpha U)(t_{n-1}),$$

with

$$(\mathcal{I}^\alpha U)(t_n) = \sum_{j=1}^n \int_{t_{j-1}}^{t_j} \omega_\alpha(t_n - s) \left(U^{j-1} + (s - t_{j-1}) \partial U^j \right) ds = \sum_{j=1}^n (\omega_{nj} U^{j-1} + \widehat{\omega}_{nj} \partial U^j).$$

Then, the numerical scheme in (9) is equivalent to

$$(13) \quad U^n + \frac{\tau_n^\alpha}{\Gamma(\alpha + 2)} \mathcal{A} U^n = U^{n-1} - \frac{\alpha \tau_n^\alpha}{\Gamma(\alpha + 2)} \mathcal{A} U^{n-1} \\ - \sum_{j=1}^{n-1} \left((\omega_{nj} - \omega_{n-1,j}) \mathcal{A} U^{j-1} + (\widehat{\omega}_{nj} - \widehat{\omega}_{n-1,j}) \mathcal{A} \partial U^j \right) + \int_{t_{n-1}}^{t_n} f(t) dt.$$

3. Error analysis. In this section, we study the error bounds from the time-stepping scheme (9). A preliminary estimate will be derived in the next lemma. For convenience, putting

$$(14) \quad \eta(t) = \eta^n = \frac{1}{\tau_n} \int_{t_{n-1}}^{t_n} \partial_t^{1-\alpha} (u - \check{u})(s) ds, \quad \text{for } t \in I_n,$$

where the piecewise linear polynomial \check{u} interpolates u at the time nodes, that is,

$$\check{u}(t) = u^{j-1} + (t - t_{j-1}) \partial u^j \quad \text{for } t_{j-1} \leq t \leq t_j \quad \text{with } 1 \leq j \leq N.$$

LEMMA 3.1. *For $1 \leq n \leq N$, we have*

$$\|U^n - u(t_n)\|^2 \leq C t_n^{1-\alpha} \sum_{j=1}^n \tau_j \|\eta^j\|_1^2.$$

Proof. From equations (8) and (9),

$$(U^j - u(t_j)) - (U^{j-1} - u(t_{j-1})) + \int_{t_{j-1}}^{t_j} \mathcal{A} \partial_t^{1-\alpha} (U - \check{u})(t) dt = \tau_j \mathcal{A} \eta^j.$$

Taking the inner product with $v := \int_{t_{j-1}}^{t_j} \partial_t^{1-\alpha} (U - \check{u}) dt = \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha (U - \check{u})' dt$ (because $U^0 - \check{u}(0) = U^0 - u_0 = 0$), and using

$$A \left(\int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha (U - \check{u})' dt, \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha (U - \check{u})' dt \right) \geq \beta \left\| \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha (U - \check{u})' dt \right\|_1^2,$$

for some positive constant β depends on Ω (due to the Poincaré inequality),

$$\tau_j \int_{t_{j-1}}^{t_j} \langle (U - \check{u})', \mathcal{I}^\alpha (U - \check{u})' \rangle dt + \beta \left\| \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha (U - \check{u})' dt \right\|_1^2 \\ \leq \tau_j \left\langle \mathcal{A} \eta^j, \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha (U - \check{u})' dt \right\rangle.$$

An application of the Cauchy-Schwarz inequality leads to

$$\tau_j \left\langle \mathcal{A}\eta^j, \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha (U - \check{u})' dt \right\rangle \leq \frac{1}{2\beta} \tau_j^2 \|\eta^j\|_1^2 + \frac{\beta}{2} \left\| \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha (U - \check{u})' dt \right\|_1^2,$$

and consequently,

$$(15) \quad \int_{t_{j-1}}^{t_j} \langle (U - \check{u})', \mathcal{I}^\alpha (U - \check{u})' \rangle dt \leq C \tau_j \|\eta^j\|_1^2.$$

Summing over the variable j ,

$$\int_0^{t_n} \langle (U - \check{u})', \mathcal{I}^\alpha (U - \check{u})' \rangle dt \leq C \sum_{j=1}^n \tau_j \|\eta^j\|_1^2.$$

Hence, using Lemma 1.1, the desired bound is obtained. \square

The current task is to estimate the candidate $\|\eta^j\|_1$ which is very delicate. The approach is novel and some new ideas are used. Starting from the fact that $(u - \check{u})(0) = 0$ (since \check{u} interpolates u at the time nodes t_n for $0 \leq n \leq N$), we observe

$$\partial_t^{1-\alpha} (u - \check{u})(t) = \mathcal{I}^\alpha (u - \check{u})'(t) = \sum_{i=1}^j \int_{t_{i-1}}^{\min\{t_i, t\}} \omega_\alpha(t-s) (u'(s) - \partial u^i) ds, \quad \text{for } t \in I_j.$$

However,

$$u(t_i) - u(t_{i-1}) = \tau_i u'(t_i) - \frac{\tau_i^2}{2} u''(t_i) + \frac{1}{2} \int_{t_{i-1}}^{t_i} (q - t_{i-1})^2 u'''(q) dq,$$

and hence, after some manipulations, one can show that

$$u'(s) - \partial u^i = e_1(s) + e_2(s) \quad \text{for } s \in I_i,$$

where

$$e_1(s) = \int_s^{t_i} (q - s) u'''(q) dq - \frac{1}{2\tau_i} \int_{t_{i-1}}^{t_i} (q - t_{i-1})^2 u'''(q) dq,$$

$$e_2(s) = (s - t_{i-1}/2) u''(t_i).$$

Thus, splitting η^j as: $\eta^j = \tau_j^{-1} (\eta_1^j + \eta_2^j)$, where

$$(16) \quad \eta_1^j = \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha e_1(t) dt \quad \text{and} \quad \eta_2^j = \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha e_2(t) dt.$$

Estimating $\|\eta_1^j\|_1$ will be the topic of the next lemma.

LEMMA 3.2. *For $1 \leq j \leq N$, we have*

$$\|\eta_1^j\|_1 \leq C \tau_j \tau_j^2 t_j^{3\alpha/2 + \sigma - 1 - 2/\gamma}, \quad \text{with } \gamma > 2/(\sigma + \alpha/2).$$

Proof. Expanding η_1^j as

$$\eta_1^j = \sum_{i=1}^j \int_{t_{j-1}}^{t_j} \int_{t_{i-1}}^{\min\{t_i, t\}} \omega_\alpha(t-s) e_1(s) ds dt.$$

From the definition of e_1 and the regularity assumption (4), for $s \in I_1$,

$$\begin{aligned} \|e_1(s)\|_1 &\leq \int_s^{t_1} (q-s) \|u'''(q)\|_1 dq + \frac{1}{2t_1} \int_0^{t_1} q^2 \|u'''(q)\|_1 dq \\ (17) \quad &\leq M \int_s^{t_1} q q^{\sigma+\alpha/2-3} dq + \frac{M}{2t_1} \int_0^{t_1} q^2 q^{\sigma+\alpha/2-3} dq \\ &\leq C \max\{s^{\sigma+\alpha/2-1}, t_1^{\sigma+\alpha/2-1}\}. \end{aligned}$$

Hence, for $j = 1$,

$$\begin{aligned} \|\eta_1^1\|_1 &\leq C \int_0^{t_1} \int_0^t \omega_\alpha(t-s) \max\{s^{\sigma+\alpha/2-1}, t_1^{\sigma+\alpha/2-1}\} ds dt \\ (18) \quad &= C \int_0^{t_1} \max\left\{\frac{\Gamma(\sigma+\alpha/2)}{\Gamma(\sigma+3\alpha/2)} t^{\sigma+3\alpha/2-1}, \omega_{\alpha+1}(t) t_1^{\sigma+\alpha/2-1}\right\} dt \\ &= C \max\left\{\frac{\Gamma(\sigma+\alpha/2)}{\Gamma(\sigma+3\alpha/2+1)} t_1^{\sigma+3\alpha/2}, \omega_{\alpha+2}(t_1) t_1^{\sigma+\alpha/2-1}\right\} \leq C \tau_1^{3\alpha/2+\sigma}. \end{aligned}$$

For the case $j \geq 2$, noting first that

$$\|\eta_1^j\|_1 \leq \int_{t_{j-1}}^{t_j} \left(\int_0^{t_1} \omega_\alpha(t-s) \|e_1(s)\|_1 ds + \sum_{i=2}^j \int_{t_{i-1}}^{\min\{t_i, t\}} \omega_\alpha(t-s) \|e_1(s)\|_1 ds \right) dt.$$

For estimating the first term on the right-hand side in the above inequality, using

$$t-s \geq t_{j-1}-s = (j-1)^\gamma \left(t_1 - \frac{s}{(j-1)^\gamma} \right) \geq (j-1)^\gamma (t_1-s) \geq (j/2)^\gamma (t_1-s),$$

and the achieved bound in (17),

$$\begin{aligned} \int_0^{t_1} \omega_\alpha(t-s) \|e_1(s)\|_1 ds &\leq C j^{\gamma(\alpha-1)} \int_0^{t_1} (t_1-s)^{\alpha-1} \max\{s^{\sigma+\alpha/2-1}, t_1^{\sigma+\alpha/2-1}\} ds \\ &= C t_j^{\alpha-1} \tau^{\gamma(1-\alpha)} \int_0^{t_1} (t_1-s)^{\alpha-1} \max\{s^{\sigma+\alpha/2-1}, t_1^{\sigma+\alpha/2-1}\} ds \\ &\leq C t_j^{\alpha-1} \tau^{\gamma(1-\alpha)} t_1^{3\alpha/2+\sigma-1} = C \tau^2 t_j^{\alpha-1} t_1^{\alpha/2+\sigma-2/\gamma} \\ &\leq C \tau^2 t_j^{3\alpha/2+\sigma-2/\gamma-1}, \quad \text{for } \gamma \geq 2/(\sigma+\alpha/2). \end{aligned}$$

On the other hand, for $s \in I_i$ with $i \geq 2$, from the definition of e_1 , the regularity assumption (4), and the time mesh property (7), we have

$$\begin{aligned} \|e_1(s)\|_1 &\leq C \tau_i \int_{t_{i-1}}^{t_i} \|u'''(q)\|_1 dq \leq C \tau_i \int_{t_{i-1}}^{t_i} q^{\sigma+\alpha/2-3} dq \\ &\leq C \tau_i^2 t_i^{\sigma+\alpha/2-3} \leq C \tau^2 t_i^{\sigma+\alpha/2-1-2/\gamma} \leq C \tau^2 s^{\sigma+\alpha/2-1-2/\gamma}. \end{aligned}$$

Thus,

$$\begin{aligned} \sum_{i=2}^j \int_{t_{i-1}}^{\min\{t_i, t\}} \omega_\alpha(t-s) \|e_1(s)\|_1 ds &\leq C\tau^2 \int_{t_1}^t (t-s)^{\alpha-1} s^{\sigma+\alpha/2-1-2/\gamma} ds \\ &\leq C\tau^2 \int_0^t (t-s)^{\alpha-1} s^{\sigma+\alpha/2-1-2/\gamma} ds \\ &\leq C\tau^2 t^{3\alpha/2+\sigma-1-2/\gamma}, \quad \text{for } \gamma > 2/(\sigma + \alpha/2). \end{aligned}$$

Gathering the above contribution and using again the time mesh property (7),

$$\|\eta_1^j\|_1 \leq C\tau_1^{3\alpha/2+\sigma} + C\tau_j\tau^2 t_j^{3\alpha/2+\sigma-1-2/\gamma}, \quad \text{for } j \geq 2 \text{ with } \gamma > 2/(\sigma + \alpha/2).$$

From this bound, and the achieved estimate in (18), the desired result is obtained. \square

It remains to estimate $\|\eta_2^j\|_1$. The technical result in the next lemma is needed.

LEMMA 3.3. *For $\gamma \geq 1$, and for a given positive sequence $\{a_i\}$, we have*

$$\sum_{i=2}^j a_i \left| \mathbf{L}^{i-1, j-1} - \frac{\tau_{i-1}^3}{\tau_i^3} \mathbf{L}^{i, j} \right| \leq C\tau t_{j-1}^{\alpha-1/\gamma} \max_{i=2}^j \left(a_i \tau_{i-1}^2 \right), \quad \text{for } 2 \leq i \leq j,$$

with

$$\mathbf{L}^{i, j} := \frac{1}{2} \int_{t_{i-1}}^{t_i} (s - t_{i-1})(t_i - s) \omega_\alpha(t_j - s) ds, \quad \text{for } 1 \leq i \leq j \leq N.$$

Proof. For $\gamma = 1$, $\mathbf{L}^{i-1, j-1} - \frac{\tau_{i-1}^3}{\tau_i^3} \mathbf{L}^{i, j} = 0$, and so, we have nothing to show. For $\gamma > 1$, from the substitution $s = \tau_i^{-1} \left((t_i - q)t_{i-2} + (q - t_{i-1})t_{i-1} \right)$, we observe

$$(19) \quad \mathbf{L}^{i-1, j-1} = \frac{1}{2} \frac{\tau_{i-1}^3}{\tau_i^3} \int_{t_{i-1}}^{t_i} (q - t_{i-1})(t_i - q) \omega_\alpha(t_{j-1} - s) dq.$$

Since $t_{j-1} - s \leq t_j - q$, $\mathbf{L}^{i-1, j-1} \geq \frac{\tau_{i-1}^3}{\tau_i^3} \mathbf{L}^{i, j}$. This leads to

$$\begin{aligned} &\sum_{i=2}^j a_i \left| \mathbf{L}^{i-1, j-1} - \frac{\tau_{i-1}^3}{\tau_i^3} \mathbf{L}^{i, j} \right| \\ &= \frac{1}{2} \sum_{i=2}^j a_i \frac{\tau_{i-1}^3}{\tau_i^3} \int_{t_{i-1}}^{t_i} (q - t_{i-1})(t_i - q) [\omega_\alpha(t_{j-1} - s) - \omega_\alpha(t_j - q)] dq \\ &\leq \frac{1}{8} \max_{i=2}^j \left(a_i \frac{\tau_{i-1}^3}{\tau_i} \right) \sum_{i=2}^j \int_{t_{i-1}}^{t_i} [\omega_\alpha(t_{j-1} - s) - \omega_\alpha(t_j - q)] dq \\ &\leq \frac{1}{8} \max_{i=2}^j \left(a_i \tau_{i-1}^2 \right) \sum_{i=2}^j \left(\frac{\tau_i}{\tau_{i-1}} \int_{t_{i-2}}^{t_{i-1}} \omega_\alpha(t_{j-1} - v) dv - \int_{t_{i-1}}^{t_i} \omega_\alpha(t_j - q) dq \right). \end{aligned}$$

A simple manipulation shows that

$$\begin{aligned} \sum_{i=2}^j \int_{t_{i-1}}^{t_i} \omega_\alpha(t_j - q) dq &= \int_{t_1}^{t_j} \omega_\alpha(t_j - q) dq \\ &= \omega_{\alpha+1}(t_j - t_1) \geq \omega_{\alpha+1}(t_{j-1}) = \sum_{i=2}^j \int_{t_{i-2}}^{t_{i-1}} \omega_\alpha(t_{j-1} - v) dv, \end{aligned}$$

and consequently,

$$\begin{aligned} \sum_{i=2}^j a_i \left| \mathbf{L}^{i-1,j-1} - \frac{\tau_{i-1}^3}{\tau_i^3} \mathbf{L}^{i,j} \right| \\ \leq \frac{1}{8} \max_{i=2}^j (a_i \tau_{i-1}^2) \sum_{i=2}^j \left(\frac{\tau_i}{\tau_{i-1}} - 1 \right) \int_{t_{i-2}}^{t_{i-1}} \omega_\alpha(t_{j-1} - q) dq. \end{aligned}$$

By the mesh properties in (7),

$$\frac{\tau_i}{\tau_{i-1}} - 1 = (\tau_i - \tau_{i-1})\tau_{i-1}^{-1} \leq C\tau^2 t_i^{1-2/\gamma} \tau^{-1} t_{i-1}^{1/\gamma-1} \leq C\tau t_{i-1}^{-1/\gamma}, \quad \text{for } i \geq 2,$$

and therefore, using $\gamma > 1$,

$$\begin{aligned} \sum_{i=2}^j \left(\frac{\tau_i}{\tau_{i-1}} - 1 \right) \int_{t_{i-2}}^{t_{i-1}} \omega_\alpha(t_{j-1} - q) dq &\leq C\tau \sum_{i=2}^j t_{i-1}^{-1/\gamma} \int_{t_{i-2}}^{t_{i-1}} \omega_\alpha(t_{j-1} - q) dq \\ &\leq C\tau \int_0^{t_{j-1}} q^{-1/\gamma} \omega_\alpha(t_{j-1} - q) dq \leq C\tau t_{j-1}^{\alpha-1/\gamma}. \end{aligned}$$

This completes the proof. \square

Now, we are ready to bound $\|\eta_2^j\|_1$.

LEMMA 3.4. *For η_2^j defined as in (16) with $j \geq 1$, we have*

$$\|\eta_2^j\|_1 \leq C\tau^2 \tau_j t_j^{3\alpha/2 + \sigma - 1 - 2/\gamma}, \quad \text{for } \gamma \geq 2/(\sigma + \alpha/2).$$

Proof. Splitting η_2^j follows by reversing the order of integration then integrating by parts,

$$\begin{aligned} \eta_2^j &= \sum_{i=1}^j u''(t_i) \int_{t_{j-1}}^{t_j} \int_{t_{i-1}}^{\min\{t_i, t\}} (s - t_{i-1/2}) \omega_\alpha(t - s) ds dt \\ &= \sum_{i=1}^{j-1} u''(t_i) \int_{t_{i-1}}^{t_i} (s - t_{i-1/2}) [\omega_{\alpha+1}(t_j - s) - \omega_{\alpha+1}(t_{j-1} - s)] ds \\ &\quad + u''(t_j) \int_{t_{j-1}}^{t_j} (s - t_{j-1/2}) \omega_{\alpha+1}(t_j - s) ds \\ &= \sum_{i=1}^{j-1} u''(t_i) [\mathbf{L}^{i,j-1} - \mathbf{L}^{i,j}] - u''(t_j) \mathbf{L}^{j,j}. \end{aligned}$$

Thus, η_2^j can be decomposed as: $\eta_2^j = -\eta_{2,1}^j - \eta_{2,2}^j - \eta_{2,3}^j$, with

$$(20) \quad \eta_{2,1}^j = \sum_{i=2}^j [u''(t_i) - u''(t_{i-1})] \mathbf{L}^{i,j},$$

$$(21) \quad \eta_{2,2}^j = \sum_{i=2}^j u''(t_{i-1}) \left(1 - \frac{\tau_{i-1}^3}{\tau_i^3} \right) \mathbf{L}^{i,j},$$

$$(22) \quad \eta_{2,3}^j = u''(t_1) \mathbf{L}^{1,j} - \sum_{i=2}^j u''(t_{i-1}) \left(\mathbf{L}^{i-1,j-1} - \frac{\tau_{i-1}^3}{\tau_i^3} \mathbf{L}^{i,j} \right).$$

By the regularity assumption in (4) and the time mesh properties in (7),

$$\begin{aligned}
\|\eta_{2,1}^j\|_1 &\leq C \sum_{i=2}^j \tau_i^2 \int_{t_{i-1}}^{t_i} \|u'''(q)\|_1 dq \int_{t_{i-1}}^{t_i} (t_j - s)^{\alpha-1} ds \\
&\leq C \sum_{i=2}^j \tau_i^3 t_i^{\sigma+\alpha/2-3} \int_{t_{i-1}}^{t_i} (t_j - s)^{\alpha-1} ds \\
(23) \quad &\leq C \tau^3 \sum_{i=2}^j t_i^{\sigma+\alpha/2-3/\gamma} \int_{t_{i-1}}^{t_i} (t_j - s)^{\alpha-1} ds \\
&\leq C \tau^3 \int_{t_1}^{t_j} s^{\sigma+\alpha/2-3/\gamma} (t_j - s)^{\alpha-1} ds \leq C \tau^3 t_j^{\sigma+3\alpha/2-3/\gamma},
\end{aligned}$$

for $\gamma \geq 2/(\sigma + \alpha/2)$. The next task is to estimate $\eta_{2,2}^j$. Seeing that

$$1 - \tau_{i-1}^3/\tau_i^3 \leq 3\tau_i^{-1}(\tau_i - \tau_{i-1}) \leq C\tau^2\tau_i^{-1}t_i^{1-2/\gamma}$$

(the third time mesh property in (7) is used here), yields

$$\begin{aligned}
\|\eta_{2,2}^j\|_1 &\leq C\tau^2 \sum_{i=2}^j \tau_i^{-1}t_i^{1-2/\gamma} \|u''(t_{i-1})\|_1 \tau_i^2 \int_{t_{i-1}}^{t_i} (t_j - s)^{\alpha-1} ds \\
(24) \quad &\leq C\tau^3 \sum_{i=2}^j \int_{t_{i-1}}^{t_i} (t_j - s)^{\alpha-1} s^{\sigma+\alpha/2-3/\gamma} ds \\
&\leq C\tau^3 \int_{t_1}^{t_j} (t_j - s)^{\alpha-1} s^{\sigma+\alpha/2-3/\gamma} ds \\
&\leq C\tau^3 t_j^{\sigma+3\alpha/2-3/\gamma}, \quad \text{for } \gamma \geq 2/(\sigma + \alpha/2).
\end{aligned}$$

To estimate $\eta_{2,3}^j$, we use again the regularity assumption in (4) and then apply Lemma 3.3 with $t_{i-1}^{\sigma-2}$ in place of a_i , and get

$$\begin{aligned}
\sum_{i=2}^j \|u''(t_{i-1})\|_1 \left| \mathbf{L}^{i-1,j-1} - \frac{\tau_{i-1}^3}{\tau_i^3} \mathbf{L}^{i,j} \right| &\leq C \sum_{i=2}^j t_{i-1}^{\sigma-2} \left| \mathbf{L}^{i-1,j-1} - \frac{\tau_{i-1}^3}{\tau_i^3} \mathbf{L}^{i,j} \right| \\
&\leq C\tau t_{j-1}^{\alpha-1/\gamma} \max_{i=2}^j \left(t_{i-1}^{\sigma+\alpha/2-2} \tau_{i-1}^2 \right) \\
&\leq C\tau^3 t_{j-1}^{\alpha-1/\gamma} \max_{i=2}^j \left(t_{i-1}^{\sigma+\alpha/2-2/\gamma} \right) \\
&\leq C\tau^3 t_{j-1}^{3\alpha/2+\sigma-3/\gamma}, \quad \text{for } \gamma \geq 2/(\sigma + \alpha/2).
\end{aligned}$$

By the definition of $\eta_{2,3}^j$ and the above contribution, we obtain

$$\begin{aligned}
\|\eta_{2,3}^j\|_1 &\leq \|u''(t_1)\|_1 \mathbf{L}^{1,j} + C\tau^3 t_{j-1}^{3\alpha/2+\sigma-3/\gamma} \\
(25) \quad &\leq C\tau_1^{\sigma+\alpha/2} \int_0^{t_1} \omega_\alpha(t_j - s) ds + C\tau^3 t_{j-1}^{3\alpha/2+\sigma-3/\gamma} \\
&\leq C\tau_1^{3\alpha/2+\sigma} + C\tau^3 t_{j-1}^{3\alpha/2+\sigma-3/\gamma}, \quad \text{for } \gamma \geq 2/(\sigma + \alpha/2).
\end{aligned}$$

Therefore, to complete the proof, combining the estimates from (23), (24) and (25), and use the inequality $\tau \leq C\tau_j t_j^{1/\gamma-1}$ (follows from the second mesh property in (7)). \square

We are ready now to estimate the pointwise error. The proof relies on the achieved results in Lemmas 3.1, 3.2 and 3.4. As mentioned earlier, the numerical results encapsulate that the imposed assumption on γ is not sharp.

THEOREM 3.5. *Let U be the time-stepping solution defined by (9) and let u be the solution of the fractional reaction-diffusion problem (1). Assume that u satisfies the regularity assumptions in (4). If the time mesh exponent γ is greater than the maximum of $\{2/(\sigma + \alpha/2), 2/(\sigma + 3\alpha/2 - 1/2)\}$ with $\sigma + 3\alpha/2 - 1/2 > 0$, then*

$$\|U^n - u(t_n)\| \leq C\tau^2 t_n^{\sigma + \alpha - 2/\gamma} \leq C\tau^2, \quad \text{for } 1 \leq n \leq N.$$

Proof. From the decomposition $\eta^j = \tau_j^{-1}(\eta_1^j + \eta_2^j)$, and the established bounds of η_1^j and η_2^j in Lemma 3.2 and Lemma 3.4, respectively,

$$\begin{aligned} \sum_{j=1}^n \tau_j \|\eta^j\|_1^2 &\leq C\tau^4 \sum_{j=1}^n \tau_j t_j^{2(3\alpha/2 + \sigma - 1 - 2/\gamma)} \\ (26) \quad &\leq C\tau^4 \int_{t_1}^{t_n} t^{2(3\alpha/2 + \sigma - 1 - 2/\gamma)} dt \\ &\leq C\tau^4 \max\{t_1^{2\sigma + 3\alpha - 4/\gamma - 1}, t_n^{2\sigma + 3\alpha - 4/\gamma - 1}\}, \quad \text{for } \gamma > 2/(\sigma + \alpha/2). \end{aligned}$$

Inserting this in the achieved bound in Lemma 3.1 and using $\gamma \geq 2/(\sigma + 3\alpha/2 - 1/2)$ will complete the proof. \square

4. Fully-discrete solution. To compute our numerical solution, we therefore seek a fully-discrete solution U_h by discretizing (9) in space via the standard Galerkin finite element method. To this end, let \mathcal{T}_h be a family of regular (conforming) triangulation of the domain $\bar{\Omega}$ and let $h = \max_{K \in \mathcal{T}_h}(\text{diam}K)$, where h_K denotes the diameter of the element K . Let $V_h \subset H_0^1(\Omega)$ denote the usual space of continuous, piecewise-linear functions on \mathcal{T}_h that vanish on $\partial\Omega$. Let $\mathcal{W}(V_h) \subset C([0, T]; V_h)$ denote the space of linear polynomials on $[t_{n-1}, t_n]$ for $1 \leq n \leq N$, with coefficients in V_h .

Taking the inner of (9) with a test function $\chi \in H_0^1(\Omega)$, and apply the first Green identity. Then, the semi-discrete $L1$ solution U satisfies

$$(27) \quad \langle U^n - U^{n-1}, \chi \rangle + \int_{t_{n-1}}^{t_n} A(\partial_t^{1-\alpha} U(t), \chi) dt = \int_{t_{n-1}}^{t_n} \langle f(t), \chi \rangle dt, \quad \text{with } U^0 = u_0,$$

Motivated by this, our fully-discrete computational solution $U_h \in \mathcal{W}(V_h)$ is defined as: for $1 \leq n \leq N$,

$$(28) \quad \langle U_h^n - U_h^{n-1}, v_h \rangle + \int_{t_{n-1}}^{t_n} A(\partial_t^{1-\alpha} U_h(t), v_h) dt = \int_{t_{n-1}}^{t_n} \langle f(t), v_h \rangle dt \quad \forall v_h \in V_h,$$

with $U_h^0 = R_h u_0$, where $R_h : H_0^1(\Omega) \rightarrow V_h$ is the Ritz projection defined by

$$A(R_h w, v_h) = A(w, v_h), \quad \forall v_h \in V_h.$$

Following the derivation used to obtain (13), the scheme in (28) is equivalent to

$$\begin{aligned} \langle U_h^n, v_h \rangle + \frac{\tau_n^\alpha}{\Gamma(\alpha + 2)} A(U_h^n, v_h) &= \langle U_h^{n-1}, v_h \rangle - \frac{\alpha \tau_n^\alpha}{\Gamma(\alpha + 2)} A(U_h^{n-1}, v_h) \\ &- A\left(\sum_{j=1}^{n-1} \left((\omega_{nj} - \omega_{n-1,j}) U_h^{j-1} + (\hat{\omega}_{nj} - \hat{\omega}_{n-1,j}) \partial U_h^j\right), v_h\right) + \int_{t_{n-1}}^{t_n} \langle f(t), v_h \rangle dt. \end{aligned}$$

For $1 \leq p \leq d_h := \dim V_h$, let $\phi_p \in V_h$ denote the p th basis function associated with the p th interior node \vec{x}_p , so that $\phi_p(\vec{x}_q) = \delta_{pq}$ and

$$U_h^n(\vec{x}) = \sum_{p=1}^{d_h} u_h^n(\vec{x}_p) \phi_p(\vec{x}).$$

We define $d_h \times d_h$ matrices: $\mathbf{M} = [\langle \phi_q, \phi_p \rangle]$, $\mathbf{G} = [A(\phi_q, \phi_p)]$, and the d_h -dimensional column vectors \mathbf{U}_h^n and \mathbf{F}^n with components $U_h^n(\vec{x}_p)$ and $\int_{t_{n-1}}^{t_n} \langle f(t), \phi_p \rangle dt$, respectively. Therefore, the fully-discrete scheme (28) has the following matrix representations:

$$\begin{aligned} \left(\mathbf{M} + \frac{\tau_n^\alpha}{\Gamma(\alpha + 2)} \mathbf{G} \right) \mathbf{U}_h^n &= \left(\mathbf{M} - \frac{\alpha \tau_n^\alpha}{\Gamma(\alpha + 2)} \mathbf{G} \right) \mathbf{U}_h^{n-1} \\ &\quad - \sum_{j=1}^{n-1} \left((\omega_{n,j} - \omega_{n-1,j}) \mathbf{G} \mathbf{U}_h^{j-1} + (\widehat{\omega}_{n,j} - \widehat{\omega}_{n-1,j}) \mathbf{G} \partial \mathbf{U}_h^j \right) + \mathbf{F}^n. \end{aligned}$$

Therefore, at each time level t_n , the numerical scheme (28) reduces to a finite square linear system, and so the existences of U_h^n follows from its uniqueness. The latter follows from the fact that both matrices \mathbf{M} and \mathbf{G} are positive definite.

Turning now into the error analysis, we introduce the following notations:

$$\theta(t) = U_h(t) - R_h \tilde{u}(t) \quad \text{and} \quad \rho(t) = u(t) - R_h u(t), \quad \text{and}.$$

Since \tilde{u} interpolates u at the time nodes, $\theta^n = U_h^n - R_h \tilde{u}(t_n) = U_h^n - R_h u(t_n)$. Thence, the pointwise time error $U_h^n - u(t_n)$ can be decomposed as

$$(29) \quad U_h^n - u(t_n) = [U_h^n - R_h u(t_n)] - [u(t_n) - R_h u(t_n)] = \theta^n - \rho^n.$$

The estimate of the second term follows easily from the Ritz projector approximation property and the first regularity assumption in (4),

$$(30) \quad \|\rho(t_n)\| \leq Ch^2 \|u(t_n)\|_2 \leq Ch^2, \quad \text{for } 0 \leq n \leq N.$$

The next duty is to estimate θ^n . From the weak formulation of problem (1);

$$\langle u(t_j) - u(t_{j-1}), \chi \rangle + \int_{t_{j-1}}^{t_j} A(\partial_t^{1-\alpha} u(t), \chi) dt = \int_{t_{j-1}}^{t_j} \langle f(t), \chi \rangle dt \quad \forall \chi \in H_0^1(\Omega),$$

the numerical scheme (28), and the decomposition in (29), we have

$$\begin{aligned} \tau_j \langle \partial \theta^j, v_h \rangle + \int_{t_{j-1}}^{t_j} A(\partial_t^{1-\alpha} (U_h - \tilde{u})(t), v_h) dt \\ = \tau_j \langle \partial \rho^n, v_h \rangle + \int_{t_{j-1}}^{t_j} A(\partial_t^{1-\alpha} (u - \tilde{u})(t), v_h) dt, \quad \forall v_h \in V_h. \end{aligned}$$

From the orthogonality property of the Ritz projection, and the definition of η in (14),

$$(31) \quad \tau_j \langle \partial \theta^j, v_h \rangle + \int_{t_{j-1}}^{t_j} A(\partial_t^{1-\alpha} \theta(t), v_h) dt = \tau_j [\langle \partial \rho^j, v_h \rangle + A(\eta^j, v_h)], \quad \forall v_h \in V_h.$$

Since $\theta^0 = U_h^0 - R_h \tilde{u}(0) = R_h u_0 - R_h u_0 = 0$, $\int_{t_{j-1}}^{t_j} \partial_t^{1-\alpha} \theta(t) dt = \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta'(t) dt$. Now, setting $v_h = \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta'(t) dt$ and applying the Poincaré inequality, then the second term in (31) is $\geq \beta \|\int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta'(t) dt\|_1^2$, for some positive constant β depends on Ω . This and the fact that $\partial \theta^j = \theta'(t)$ (constant in time) for $t \in I_j$, lead to

$$\begin{aligned} \tau_j \int_{t_{j-1}}^{t_j} \langle \theta', \mathcal{I}^\alpha \theta' \rangle dt + \beta \left\| \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta' dt \right\|_1^2 \\ \leq \tau_j \left\langle \partial \rho^j, \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta' dt \right\rangle + \tau_j A(\eta^j, \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta' dt). \end{aligned}$$

By the Cauchy-Schwarz inequality, the last term is

$$\leq \frac{1}{2\beta} \tau_j^2 \|\eta^j\|_1^2 + \frac{\beta}{2} \left\| \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta' dt \right\|_1^2,$$

and consequently,

$$(32) \quad \tau_j \int_{t_{j-1}}^{t_j} \langle \theta', \mathcal{I}^\alpha \theta' \rangle dt + \frac{\beta}{2} \left\| \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta' dt \right\|_1^2 \leq \tau_j \int_{t_{j-1}}^{t_j} \langle \tilde{\rho}', \mathcal{I}^\alpha \theta' \rangle dt + C \tau_j^2 \|\eta^j\|_1^2,$$

where $\tilde{\rho}(t) = \rho^{j-1} + (t - t_{j-1})\partial \rho^j$ for $t \in I_j$. Dividing both sides by τ_j , and then, summing over the variable j and using the inequality

$$(33) \quad \int_0^{t_n} \langle \tilde{\rho}', \mathcal{I}^\alpha \theta' \rangle dt \leq \frac{1}{2(1-\alpha)^2} \int_0^{t_n} \langle \tilde{\rho}', \mathcal{I}^\alpha \tilde{\rho}' \rangle dt + \frac{1}{2} \int_0^{t_n} \langle \theta', \mathcal{I}^\alpha \theta' \rangle dt,$$

(Lemma 1.2 is used here), we reach

$$\int_0^{t_n} \langle \theta', \mathcal{I}^\alpha \theta' \rangle dt \leq \frac{1}{(1-\alpha)^2} \int_0^{t_n} \langle \tilde{\rho}', \mathcal{I}^\alpha \tilde{\rho}' \rangle dt + C \tau_j \|\eta^j\|_1^2.$$

Thanks to Lemma 1.1,

$$(34) \quad \|\theta^n\|^2 \leq C t_n^{1-\alpha} \left(\int_0^{t_n} |\langle \tilde{\rho}', \mathcal{I}^\alpha \tilde{\rho}' \rangle| dt + \sum_{j=1}^n \tau_j \|\eta^j\|_1^2 \right).$$

To estimate $\int_0^{t_n} |\langle \tilde{\rho}', \mathcal{I}^\alpha \tilde{\rho}' \rangle| dt$, split it as (recall that $\tilde{\rho}'(t) = \partial \rho^j$ on I_j)

$$(35) \quad \begin{aligned} \int_0^{t_n} |\langle \tilde{\rho}'(t), \mathcal{I}^\alpha \tilde{\rho}'(t) \rangle| dt &\leq \|\partial \rho^1\|^2 \int_0^{t_1} \int_0^t \omega_\alpha(t-s) ds dt \\ &+ \sum_{j=2}^n \|\partial \rho^j\| \|\partial \rho^1\| \int_{t_{j-1}}^{t_j} \int_0^{t_1} \omega_\alpha(t-s) ds dt \\ &+ \sum_{j=2}^n \|\partial \rho^j\| \sum_{i=2}^j \|\partial \rho^i\| \int_{t_{j-1}}^{t_j} \int_{t_{i-1}}^{\min\{t_i, t\}} \omega_\alpha(t-s) ds dt. \end{aligned}$$

By the definition of the function ρ , the Ritz projection error bound in (30) with u' in place of u , and the regularity assumption (4), we obtain

$$(36) \quad \begin{aligned} \|\partial \rho^j\| &= \tau_j^{-1} \left\| \int_{t_{j-1}}^{t_j} (R_h u' - u')(s) ds \right\| \\ &\leq C h^2 \tau_j^{-1} \int_{t_{j-1}}^{t_j} \|u'(s)\|_2 ds \leq C h^2 \tau_j^{-1} \int_{t_{j-1}}^{t_j} s^{\sigma-1} ds, \quad \text{for } j \geq 1. \end{aligned}$$

If $\sigma - 1 \geq 0$ (which might not be practically the case), then $\|\partial\rho^j\| \leq Ch^2t_j^{\sigma-1}$. Thus,

$$(37) \quad \int_0^{t_n} |\langle \check{\rho}', \mathcal{I}^\alpha \check{\rho}' \rangle| dt \leq Ch^4 t_n^{2\sigma-2} \int_0^{t_n} \int_0^t \omega_\alpha(t-s) ds dt \leq Ch^4 t_n^{2\sigma+\alpha-1}, \quad \text{for } \sigma \geq 1.$$

Now, turning into the case $\sigma - 1 < 0$, which is probably more interesting. Assuming that $\sigma > (1 - \alpha)/2$, a similar bound will be achieved next, see (38). Using (36), the first term on the right-hand side of (35) is bounded by

$$Ch^4 \tau_1^{-2} \left(\int_0^{t_1} s^{\sigma-1} ds \right)^2 \omega_{\alpha+2}(t_1) \leq Ch^4 t_1^{2\sigma+\alpha-1}.$$

Using (36) and the first time mesh property in (7), the second candidate on the right-hand side of (35) is

$$\begin{aligned} &\leq Ch^4 \sum_{j=2}^n t_j^{\sigma-1} \frac{1}{\tau_1} \int_0^{t_1} s^{\sigma-1} ds \int_{t_{j-1}}^{t_j} \int_0^{t_1} \omega_\alpha(t-s) ds dt \\ &\leq Ch^4 \sum_{j=2}^n (t_1 t_j)^{\sigma-1} \int_{t_{j-1}}^{t_j} \int_0^{t_1} \omega_\alpha(t-s) ds dt \\ &\leq Ch^4 \sum_{j=2}^n \int_{t_{j-1}}^{t_j} t^{\sigma-1} \int_0^{t_1} s^{\sigma-1} \omega_\alpha(t-s) ds dt \\ &\leq Ch^4 \int_{t_1}^{t_n} t^{\sigma-1} \int_0^t s^{\sigma-1} \omega_\alpha(t-s) ds dt \leq Ch^4 \int_{t_1}^{t_n} t^{2\sigma+\alpha-2} dt, \end{aligned}$$

while, the last term in (35) is

$$\begin{aligned} &\leq Ch^4 \sum_{j=2}^n t_j^{\sigma-1} \sum_{i=2}^j \frac{1}{\tau_i} \int_{I_i} s^{\sigma-1} ds \int_{t_{j-1}}^{t_j} \int_{t_{i-1}}^{\min\{t_i, t\}} \omega_\alpha(t-s) ds dt \\ &\leq Ch^4 \sum_{j=2}^n t_j^{\sigma-1} \sum_{i=2}^j t_i^{\sigma-1} \int_{t_{j-1}}^{t_j} \int_{t_{i-1}}^{\min\{t_i, t\}} \omega_\alpha(t-s) ds dt \\ &\leq Ch^4 \sum_{j=2}^n \sum_{i=1}^j \int_{t_{j-1}}^{t_j} t^{\sigma-1} \int_{t_{i-1}}^{\min\{t_i, t\}} s^{\sigma-1} \omega_\alpha(t-s) ds dt \\ &\leq Ch^4 \int_{t_1}^{t_n} t^{\sigma-1} \int_0^t s^{\sigma-1} \omega_\alpha(t-s) ds dt \leq Ch^4 \int_{t_1}^{t_n} t^{2\sigma+\alpha-2} dt. \end{aligned}$$

Therefore, gathering the above estimates, we conclude that

$$(38) \quad \int_0^{t_n} |\langle \check{\rho}', \mathcal{I}^\alpha \check{\rho}' \rangle| dt \leq Ch^4 t_n^{2\sigma+\alpha-1}, \quad \text{for } (1 - \alpha)/2 < \sigma < 1.$$

From the decomposition (29), the Ritz projection in (30), the inequality in (34), the achieved bounds in (26) and (37), and the above estimate, the error result in the next convergence theorem holds true. It is claimed that for a sufficiently time-graded mesh, the proposed fully-discrete scheme is second-order accurate in both time and space. The numerical results in the forthcoming section confirm that the imposed assumption on the time mesh exponent γ is pessimistic. Furthermore, these results

also illustrate $O(h^2)$ -rates of convergence in space, although the imposed condition $\sigma > (1 - \alpha)/2$ in the next theorem is not satisfied. Indeed, for the semi-discrete Galerkin method in space for problem (1), an $O(h^2)$ -rate of convergence was carried out without this assumption [13].

THEOREM 4.1. *Let U_h be the numerical solution defined by (28) and let u be the solution of the fractional reaction-diffusion problem (1). Assume that u satisfies the regularity assumptions in (4) with $\sigma > (1 - \alpha)/2$. If the time mesh exponent $\gamma > \max\{2/(\sigma + \alpha/2), 2/(\sigma + 3\alpha/2 - 1/2)\}$, then*

$$\|U_h^n - u(t_n)\| \leq C(\tau^2 + h^2), \quad \text{for } 1 \leq n \leq N.$$

We end this section with the following remark.

Remark 4.2. Due to the use of the inequality in (33), the coefficient C in (34) blows up as $\alpha \rightarrow 1^-$. To control this phenomena, Lemma 1.2 (and consequently, the inequality in (33)) should be avoided. Since $\rho'(t) = \partial\rho^j$ for $t \in I_j$, an application of the Cauchy-Schwarz inequality yields

$$\tau_j \int_{t_{j-1}}^{t_j} \langle \rho', \mathcal{I}^\alpha \theta' \rangle dt = \left\langle \tau_j \partial\rho^j, \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta' dt \right\rangle \leq C\tau_j^2 \|\partial\rho^j\|^2 + \frac{\beta}{2} \left\| \int_{t_{j-1}}^{t_j} \mathcal{I}^\alpha \theta'(t) dt \right\|_1^2.$$

Substitute this in (32) gives

$$\int_{t_{j-1}}^{t_j} \langle \theta', \mathcal{I}^\alpha \theta' \rangle dt \leq C\tau_j \|\partial\rho^j\|^2 + C\tau_j \|\eta^j\|_1^2.$$

Summing over j , follows by using Lemma 1.1 with θ in place of ϕ , we notice that

$$\|\theta^n\|^2 \leq C t_n^{1-\alpha} \left(\sum_{j=1}^n \tau_j \|\partial\rho^j\|^2 + \sum_{j=1}^n \tau_j \|\eta^j\|_1^2 \right),$$

where the constant C in the above bound does not blowup as $\alpha \rightarrow 1^-$.

The remaining exercise is to estimate $\sum_{j=1}^n \tau_j^{-1} \|\partial\rho^j\|^2$. From (36),

$$\begin{aligned} \sum_{j=1}^n \tau_j \|\partial\rho^j\|^2 &\leq Ch^4 \sum_{j=1}^n \tau_j^{-1} \left(\int_{t_{j-1}}^{t_j} s^{\sigma-1} ds \right)^2 \leq Ch^4 \sum_{j=1}^n \int_{t_{j-1}}^{t_j} s^{2\sigma-2} ds \\ &= Ch^4 \int_0^{t_n} s^{2\sigma-2} ds \leq Ch^4 t_n^{2\sigma-1}, \quad \text{for } \sigma > 1/2. \end{aligned}$$

For $\sigma = 1/2$, these steps can be slightly adjusted to show an $O(h^4)$ bound of the above term, but with a logarithmic coefficient $\log(t_n/t_1)$ for $n \geq 2$.

5. Numerical results. To support the achieved theoretical convergence results in Theorems 3.5 and 4.1, this section is devoted to perform some numerical experiments (on a typical test problem). In the fractional model problem (1), we choose $u_0(x, y) = x(1 - x)$, $\kappa_\alpha = d = 1$, and $f = 0$. The time and space domains are chosen to be the intervals $[0, 1]$ and $(0, 1)$, respectively. Separation of variables yields the series representation of the solution:

$$(39) \quad u(x, t) = 8 \sum_{m=0}^{\infty} \lambda_m^{-3} \sin(\lambda_m x) E_\alpha(-\lambda_m^2 t^\alpha), \quad \lambda_m := (2m + 1)\pi - 1,$$

M	$\gamma = 1$		$\gamma = 2$		$\gamma = 3$		$\gamma = 4$	
20	3.40e-02		1.09e-02		2.15e-03		8.02e-04	
40	2.78e-02	0.292	5.16e-03	1.083	7.05e-04	1.607	2.13e-04	1.911
80	2.19e-02	0.346	2.34e-03	1.142	2.46e-04	1.518	5.57e-05	1.935
160	1.65e-02	0.402	1.10e-03	1.085	8.66e-05	1.509	1.44e-05	1.951
320	1.20e-02	0.458	5.44e-04	1.019	3.05e-05	1.505	3.70e-06	1.962
640	8.48e-03	0.506	2.71e-04	1.001	1.08e-05	1.503	9.44e-07	1.972

TABLE 1

Errors and convergence rates (r_t) for $\alpha = 0.4$ and for different choices of γ .

M	$\gamma = 1$		$\gamma = 2$		$\gamma = 2.5$		$\gamma = 3$	
20	2.51e-02		2.21e-03		8.26e-04		6.50e-04	
40	1.50e-02	0.748	7.60e-04	1.540	2.12e-04	1.964	1.65e-04	1.979
80	8.32e-03	0.846	2.66e-04	1.513	5.44e-05	1.960	4.17e-05	1.982
160	4.53e-03	0.879	9.36e-05	1.509	1.46e-05	1.897	1.05e-05	1.987
320	2.53e-03	0.840	3.30e-05	1.505	3.93e-06	1.893	2.65e-06	1.991
640	1.47e-03	0.779	1.16e-05	1.503	1.06e-06	1.892	6.64e-07	1.995

TABLE 2

Errors and convergence rates (r_t) for $\alpha = 0.6$ and for different choices of γ .

where $E_\alpha(t) := \sum_{p=0}^{\infty} \frac{t^p}{\Gamma(\alpha p + 1)}$ is the Mittag-Leffler function.

The initial data $u_0 \in \dot{H}^{2.5^-}(\Omega) \cap H_0^1(\Omega)$. Thus, as expected from the regularity analysis in [18, 22], the regularity properties in (4) hold true for $\sigma = \alpha^-/4$.

For the numerical illustration of the convergence rates from the time-stepping $L1$ scheme, we refine the spatial (uniform) mesh size h so that the time errors are dominant. Therefore, by Theorems 3.5 and 4.1, we expect to observe $O(\tau^2)$ -rates of convergence for $\gamma > \max\{2/(\sigma + \alpha/2), 2/(\sigma + 3\alpha/2 - 1/2)\} = \max\{8/(3\alpha^-), 8/(7\alpha^- - 2)\}$, with $\sigma + 3\alpha/2 - 1/2 > 0$. However, the results in Tables 1–3 are more optimistic, $O(\tau^2)$ -rates were observed for $\gamma \geq 2/(\sigma + \alpha) = 8/(5\alpha^-)$, for different values of α . Moreover, these results confirm that the condition $\sigma + 3\alpha/2 - 1/2 > 0$ is not necessary.

In all tables and figures, we evaluated the series solution u in (39) of problem (1) by truncating the Fourier series in (39) after 60 terms. To measure the error in the numerical solution, we computed

$$E_{N,M} := \max_{1 \leq n \leq N} \|U_h^n - u(t_n)\|,$$

where N is the number of time subintervals, while M is the number of uniform space mesh elements. Noting that, the spatial L_2 -norm was evaluated using the two-point Gauss quadrature rule on the finest spatial mesh. The convergence rates r_t (in time) and r_x (in space) were calculated from the relations

$$r_t \approx \log_2 \left(E_{N,M} / E_{2N,M} \right), \quad \text{when } h^{r_x} \ll \tau^{r_t},$$

$$r_x \approx \log_2 \left(E_{N,M} / E_{N,2M} \right), \quad \text{when } \tau^{r_t} \ll h^{r_x}.$$

For the graphical interpretation, we fixed $N = 160$ and $M = 1200$, so the time error is dominant. Figure 1 shows how the error on uniform and nonuniform time meshes varies with t for various choices of α , using a log scale.

M	$\gamma = 1$		$\gamma = 1.5$		$\gamma = 2$	
20	9.7410e-03		1.8813e-03		5.4226e-04	
40	4.2516e-03	1.1961	6.7825e-04	1.4719	1.3563e-04	1.9993
80	2.0954e-03	1.0207	2.3983e-04	1.4998	3.4030e-05	1.9948
160	1.0687e-03	9.7134	8.4803e-05	1.4998	8.5585e-06	1.9914
320	5.3632e-04	9.9475	2.9991e-05	1.4996	2.1776e-06	1.9746

TABLE 3

Errors and convergence rates (r_t) for $\alpha = 0.8$ and for different choices of γ .

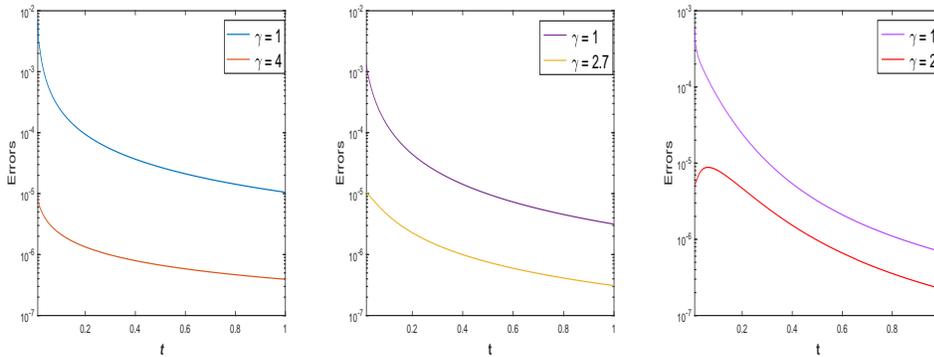


FIG. 1. The error $\|U_h^n - u(t_n)\|$ as a function of t_n . The fractional exponent $\alpha = 0.4$ in the left figure, while $\alpha = 0.6$ in the middle one, and $\alpha = 0.8$ in the right figure.

To demonstrate the $O(h^2)$ -rates from the spatial discretization by Galerkin finite elements, the time mesh size is refined so that the errors in space are dominant. The expected convergence orders are displayed in Table 4 for $\alpha = 0.3, 0.5$, and 0.8 . These results also illustrate that the condition $\sigma > (1 - \alpha)/2$ in Theorem 4.1 is not necessary. This condition holds true if $\alpha > 2/3$ because $\sigma = \alpha^-/4$, however an $O(h^2)$ -rate was observed despite α not being greater than $2/3$.

6. Concluding remarks. An $L1$ time-stepping scheme for a time-fractional diffusion equation is developed. Over a sufficiently time-graded mesh, it is claimed that the proposed scheme is second-order accurate. Later on, our $L1$ scheme is combined with the standard Galerkin finite elements for the spatial discretization. The error analysis of the induced fully-discrete scheme is studied. The delivered numerical tests confirmed that the achieved time-space convergence rates are sharp, but the time-mesh exponent γ can be further relaxed. Due to several difficulties, improving the choice of γ is beyond the scope of this work, it will be a subject of future research.

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M	$\alpha = 0.3$		$\alpha = 0.5$		$\alpha = 0.8$	
10	8.4612e-04		8.4612e-04		8.4612e-04	
20	1.9932e-04	2.0858	1.9932e-04	2.0858	1.9932e-04	2.0858
40	4.8140e-05	2.0498	4.8140e-05	2.0498	4.8140e-05	2.0498
80	1.1795e-05	2.0291	1.1449e-05	2.0720	1.1449e-05	2.0720
160	3.0940e-06	1.9306	2.9063e-06	1.9780	2.7481e-06	2.0587

TABLE 4

Errors and the spatial convergence rates r_x for different values of α .

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