

TIME-SPLITTING SCHEMES FOR FRACTIONAL DIFFERENTIAL EQUATIONS I: SMOOTH SOLUTIONS*

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Abstract. We propose three time-splitting schemes for nonlinear time-fractional differential equations with smooth solutions, where the order of the fractional derivative is $0 < \alpha < 1$. While one of the schemes is of order α , the other two schemes are of order $1 + \alpha$ and $2 - \alpha$ and thus they can be combined to provide flexible numerical methods with convergence order no less than $3/2$. We prove the convergence and stability of the proposed schemes. Numerical examples illustrate the flexibility and the efficiency of these time-splitting schemes and show that they work for multirate and stiff time-fractional differential systems effectively.

Key words. time-fractional derivatives, multirate systems, stiff systems

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1. Introduction. We aim at constructing efficient splitting methods for time-fractional differential equations with smooth solutions. The motivation of this work is to solve stiff systems of fractional differential equations and also nonlinear fractional differential equations. Though there are some explicit methods for stiff ordinary differential equations and stochastic differential equations [21, 24], most of the numerical methods for fractional stiff systems and nonlinear problems are implicit, see [4, 17, 19, 35] for trapezoidal rule, [13] for fractional Adams–Moulton methods, and [23, 39] for fractional backward differentiation formula. All these methods should be accompanied by efficient nonlinear iterative solvers. To solve nonlinear problems at reasonable computational costs, various numerical methods have been proposed: predictor-corrector methods (see [6, 7, 8, 9, 17, 25, 37, 43]), implicit-explicit (IMEX) schemes (also known as semi-implicit schemes, linearly implicit schemes) (see [38]), and some linearization of the implicit trapezoidal rule [41].

For stiff systems, especially for multiscale problems, splitting methods (also known as operator splitting methods, split-up methods, or fractional-step methods (see [20, 22, 32])) are more preferable as we can split these problems into simpler subsystems so that we can solve each subsystem with optimal numerical schemes. For example, one common splitting strategy for stiff/nonlinear problems is to split the problems into nonstiff/nonlinear parts and stiff/linear parts, and subsequently solve the nonstiff/nonlinear parts with explicit methods and the rest with implicit methods. In this case, splitting methods are very similar to IMEX methods. However, splitting

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methods are more flexible as they allow substepping of different subsystems; see [1] for integer-order equations, where the fast varying scales are solved with smaller steps. See also Example 4.3 for a splitting scheme with substepping for a stiff time-fractional differential equation.

Splitting methods themselves are in some sense preprocessing methods and require further time discretization. All the aforementioned numerical methods can be applied in time as well as many other discretization methods, such as Euler methods [15, 27, 34], Runge-Kutta methods [3, 28]), the fractional Adam–Bashforth method [16], and exponential integrator methods [18], etc. As in the context of numerical methods of differential equations of integer order, the splitting methods can be used in physical space as well; see [2, 5, 36, 40, 42, 44]. However, in this paper, we only consider time-splitting methods for time-fractional differential equations.

Though splitting methods are standard and powerful in solving differential equations of integer order, it is not straightforward to apply these methods to fractional differential equations because of the nonlocal nature of fractional differential equations. Consider the following scalar fractional differential equation

$$(1.1) \quad ({}^C D_0^\alpha u)(t) = \lambda u(t) + \sigma u(t), \quad \lambda, \sigma \in \mathbb{C}, \quad 0 < t \leq T,$$

where $u(0) = u_0$ and $({}^C D_0^\alpha u)(t)$, $0 < \alpha < 1$, is the Caputo derivative defined by

$$(1.2) \quad ({}^C D_a^\alpha g)(t) = (I_a^{1-\alpha} g')(t), \quad (I_a^\alpha g)(t) = \frac{1}{\Gamma(\alpha)} \int_a^t \frac{g(\tau)}{(t-\tau)^{1-\alpha}} d\tau, \quad t > a.$$

Suppose that we split this equation as we do for integer-order differential equations, e.g., for one step, $0 \leq t \leq h$,

$$\begin{aligned} ({}^C D_0^\alpha \bar{u})(t) &= \lambda \bar{u}(t), \quad \bar{u}(0) = u_0, \\ ({}^C D_0^\alpha \tilde{u})(t) &= \sigma \tilde{u}(t), \quad \tilde{u}(0) = \bar{u}(h). \end{aligned}$$

The splitting error is $O(h^{2\alpha})$, i.e.,

$$(1.3) \quad \begin{aligned} u(h) - \tilde{u}(h) &= u_0 \left[\sum_{k=0}^{\infty} \frac{(\lambda + \sigma)^k h^{k\alpha}}{\Gamma(1 + k\alpha)} - \sum_{k=0}^{\infty} \frac{(\lambda h^\alpha)^k}{\Gamma(1 + k\alpha)} \sum_{k=0}^{\infty} \frac{(\sigma h^\alpha)^k}{\Gamma(1 + k\alpha)} \right] \\ &= u_0 \left[\frac{2\lambda\sigma}{\Gamma(1 + 2\alpha)} - \frac{\lambda\sigma}{(\Gamma(1 + \alpha))^2} \right] h^{2\alpha} + O(h^{3\alpha}), \quad 0 < \alpha < 1. \end{aligned}$$

Thus, when α is close to zero, the obtained splitting scheme has low convergence order even in one step. The slow convergence can be explained as follows. When we split the fractional differential equation as above, we oversimplify the strongly nonlocal interactions of \tilde{u} and \bar{u} by considering the initial condition, i.e., only locally at $t = h$, while the solution at the time h to the integral equation (1.1) has a strongly nonlocal dependence on the solution at time $0 \leq t < h$.

The main contribution of this paper is to provide a convergent splitting strategy for time-fractional differential equations and subsequently develop some fully discrete time-splitting schemes. The first proposed splitting scheme is based on an integral formulation of the considered equations using a modified trapezoidal rule and the convergence order is $1 + \alpha$. The second splitting scheme is also based on an integral formulation and the convergence order is α . Since, for small α , the convergence orders of the first two schemes are either close to 1 or 0, we are motivated to develop

another splitting scheme of order $2 - \alpha$. This third splitting scheme is based on the so-called $L1$ discretization of fractional derivatives employed in [27, 34]. Thus, we can achieve a convergence order $3/2$ for every $0 < \alpha < 1$ if we choose the first and the third splitting schemes properly.

Compared to fully implicit schemes, the proposed time-splitting schemes do not require any nonlinear iterative solvers like fixed-point iteration or Newton iteration methods. The two main time-splitting schemes (the first and the third) we propose are $A(\frac{\alpha\pi}{2})$ -stable and have better stability than explicit methods. We numerically compare our splitting methods with the classical predictor-corrector method from [8] and we find that the splitting methods outperform the classical predictor-corrector scheme when stiff time-fractional differential equations systems and nonlinear time-fractional differential equations are considered.

In this work, we assume that either the solutions to the underlying equations have at least bounded first two derivatives or smooth forcing terms; see Remark 2.3 for discussions on regularity. However, these assumptions may not hold for some time-fractional differential equations; see, for example, [23, 39] and Remark 2.9 in section 2. We focus here on how to develop splitting schemes and the splitting errors. In subsequent work, we will develop splitting schemes without these assumptions.

The rest of the paper is organized as follows. We present splitting strategies for time-fractional differential equations and formulate fully discrete time-splitting schemes in section 2. We also provide convergence rates of the proposed splitting schemes, the proofs of which can be found in section 5. In section 3, we discuss the linear stability of the proposed schemes. In section 4 we present numerical examples to illustrate the computational flexibility and verify our error estimates. We conclude in section 6 and discuss our future work.

2. Time-splitting methods for time-fractional differential equations.

We consider the following nonlinear time-fractional differential system

$$(2.1) \quad ({}^C D_0^\alpha u)(t) = Au(t) + f(t, u(t)), \quad t \in (0, T], \quad u(0) = u_0,$$

where $0 < \alpha < 1$, A is an $m \times m$ real-valued matrix, $f : [0, T] \times \mathbb{R}^m \rightarrow \mathbb{R}^m$. In the rest of the paper, we suppose that f is continuous and satisfies the Lipschitz condition with respect to its second argument on a suitable domain G :

$$(2.2) \quad |f(t, u_1) - f(t, u_2)| \leq K|u_1 - u_2| \quad \forall u_1, u_2 \in G,$$

where K is a positive constant only dependent on the domain G and $|\cdot|$ denotes the Euclidean norm.

In the following text, we will use the following notation extensively:

$$(2.3) \quad \begin{aligned} ({}_{[s]}^C D_a^\alpha g)(t) &= \frac{1}{\Gamma(1-\alpha)} \int_a^t \frac{g'(\tau) d\tau}{(s-\tau)^\alpha}, \\ ({}_{[s]} I_a^\alpha g)(t) &= \frac{1}{\Gamma(\alpha)} \int_a^t \frac{g(\tau)}{(s-\tau)^{1-\alpha}} d\tau, \\ ({}_{[s]} I_a^\alpha f)(t, u(t)) &= \frac{1}{\Gamma(\alpha)} \int_a^t \frac{f(\tau, u(\tau))}{(s-\tau)^{1-\alpha}} d\tau. \end{aligned}$$

2.1. Time-splitting based on an integral formulation. To derive splitting schemes, we rewrite (2.1) in integral form:

$$(2.4) \quad u(t) = u(0) + A(I_0^\alpha u)(t) + (I_0^\alpha f)(t, u(t)), \quad 0 \leq t \leq T,$$

where we applied the operator $(I_0^\alpha \cdot)(t)$ on both sides of (2.1), used the identity $(I_a^\alpha {}^C D_a^\alpha u)(t) = u(t) - u(a)$ [33], and

$$(I_0^\alpha f)(t, u(t)) := \frac{1}{\Gamma(\alpha)} \int_0^t \frac{f(\tau, u(\tau))}{(t-\tau)^{1-\alpha}} d\tau.$$

We will use a uniform partition of time interval $[0, T]$, i.e., $t_n = nh, 0 \leq n \leq N$ with $h = T/N$.

Based on the additivity of fractional integrals over intervals (see [7]), we rewrite (2.4) over $(t_{n-1}, t_n]$ ($n \geq 1$) as

$$(2.5) \quad u(t) = u(t_0) + I_{t_{n-1}}^\alpha Au(t) + ({}_{[t]}I_{t_0}^\alpha Au)(t_{n-1}) + (I_{t_0}^\alpha f)(t, u(t)).$$

To derive a splitting method, we assume that the solution over the time interval $[0, t_{n-1}]$ is known and we denote it by $\tilde{u}(t), 0 \leq t \leq t_{n-1}$. We also define

$$(2.6) \quad \bar{u}(t) = \tilde{u}(t_{n-1}) + ({}_{[t]}I_{t_0}^\alpha A\tilde{u})(t_{n-1}) + (I_{t_{n-1}}^\alpha A\bar{u})(t), \quad t_{n-1} < t \leq t_n.$$

Introduce the notation for “initial value” of \bar{u} at t_{n-1} as

$$(2.7) \quad \tilde{u}^c(t_{n-1}) = \tilde{u}(t_{n-1}) + ({}_{[t]}I_{t_0}^\alpha A\tilde{u})(t_{n-1}).$$

Then (2.6) reads

$$(2.8) \quad \bar{u}(t) = \tilde{u}^c(t_{n-1}) + (I_{t_{n-1}}^\alpha A\bar{u})(t), \quad t_{n-1} < t \leq t_n.$$

With (2.5) and (2.6), we have

$$(2.9) \quad \tilde{u}(t) = \bar{u}^c(t_n) + (I_{t_0}^\alpha f)(t, \tilde{u}(t)), \quad t_{n-1} < t \leq t_n,$$

where we denote

$$(2.10) \quad \bar{u}^c(t_n) = \bar{u}(t) - \tilde{u}(t_{n-1}) + u(t_0) - (I_{t_{n-1}}^\alpha A(\bar{u} - \tilde{u}))(t).$$

From here, we can repeat the above procedure to obtain the solution $\tilde{u}(t)$ for $t \in (t_n, t_{n+1}]$. It can be readily checked that (2.8)–(2.10) have unique solutions as long as (2.4) has a unique solution.

We note that there is no splitting error in the above formulation, which can be readily checked that (2.7)–(2.10) can lead to exactly (2.5). Correspondingly, convergence orders of numerical schemes based on (2.7)–(2.10) depend on the convergence orders of numerical schemes applied in each subequation in (2.7)–(2.10). In splitting methods, different numerical schemes can be used in different subequations of (2.7)–(2.10) while the IMEX methods do not have this flexibility. We note that various time discretization schemes can be used, for example, those introduced in section 1.

Taking $t = t_n$, it follows from (2.7)–(2.10) that

$$(2.11) \quad \bar{u}(t_n) = \tilde{u}^c(t_{n-1}) + (I_{t_{n-1}}^\alpha A\bar{u})(t_n),$$

$$(2.12) \quad \tilde{u}^c(t_{n-1}) = \tilde{u}(t_{n-1}) + ({}_{[t_n]}I_{t_0}^\alpha A\tilde{u})(t_{n-1}), \quad \tilde{u}_0 = u_0,$$

$$(2.13) \quad \tilde{u}(t_n) = \bar{u}^c(t_n) + (I_{t_0}^\alpha f)(t_n, \tilde{u}(t_n)),$$

$$(2.14) \quad \bar{u}^c(t_n) = \bar{u}(t_n) - \tilde{u}(t_{n-1}) + u(t_0) - (I_{t_{n-1}}^\alpha A(\bar{u} - \tilde{u}))(t_n).$$

Now we derive fully discrete time-splitting schemes with further discretization of (2.11)–(2.14). To ensure stability, we approximate the fractional integral in (2.11) and

(2.14) implicitly. Applying the weighted right-rectangle rule (see [10, Appendix C]) in (2.14) leads to

$$\begin{aligned} \bar{u}^c(t_n) &\approx \bar{u}(t_n) - \tilde{u}(t_{n-1}) + u(t_0) - \frac{1}{\Gamma(\alpha)} \int_{t_{n-1}}^{t_n} \frac{A(\bar{u}(t_n) - \tilde{u}(t_n))}{(t_n - \tau)^{1-\alpha}} d\tau \\ &= \bar{u}(t_n) - \tilde{u}(t_{n-1}) + u(t_0) - \frac{Ah^\alpha}{\Gamma(1 + \alpha)} (\bar{u}(t_n) - \tilde{u}(t_n)). \end{aligned}$$

Substituting the above formula into (2.13), using \bar{u}_n and \tilde{u}_n in place of $\bar{u}(t_n)$ and $\tilde{u}(t_n)$, respectively, we obtain that

$$(2.15) \quad C_h^\alpha \tilde{u}_n = C_h^\alpha \bar{u}_n + u_0 - \tilde{u}_{n-1} + (I_{t_0}^\alpha f)(t_n, \tilde{u}(t_n)).$$

We further denote all known information in (2.15) by \bar{u}_n^c and get

$$(2.16) \quad C_h^\alpha \tilde{u}_n = \bar{u}_n^c + (I_{t_{n-1}}^\alpha f)(t_n, \tilde{u}(t_n)),$$

$$(2.17) \quad \bar{u}_n^c = C_h^\alpha \bar{u}_n + u_0 - \tilde{u}_{n-1} + ([t_n]I_{t_0}^\alpha f)(t_{n-1}, \tilde{u}(t_{n-1})),$$

where $C_h^\alpha = I - A \frac{h^\alpha}{\Gamma(1+\alpha)}$. Subsequently, we employ a weighted trapezoidal rule to approximate the integral in (2.12), and a weighted midpoint rule with $\tilde{u}(t_{j-\frac{1}{2}}) \approx \frac{1}{2}(\tilde{u}(t_{j-1}) + \tilde{u}(t_j))$ to approximate the integral in (2.17). Similarly, we use the weighted right-rectangle rule for the integral in (2.11), and the weighted left-rectangle rule for the integral in (2.16); see [26]. We then obtain the following time-splitting scheme (TS-I):

$$(2.18) \quad \bar{u}_n = \tilde{u}_{n-1}^c + \frac{Ah^\alpha}{\Gamma(1 + \alpha)} \bar{u}_n, \quad n = 1, 2, \dots, N,$$

$$(2.19) \quad \tilde{u}_{n-1}^c = \tilde{u}_{n-1} + \frac{Ah^\alpha}{2\Gamma(1 + \alpha)} \sum_{j=1}^{n-1} w_{n,j}^\alpha (\tilde{u}_{j-1} + \tilde{u}_j), \quad \tilde{u}_0 = u_0,$$

$$(2.20) \quad C_h^\alpha \tilde{u}_n = \bar{u}_n^c + \frac{h^\alpha}{\Gamma(1 + \alpha)} f(t_{n-1}, \tilde{u}_{n-1}), \quad n = 1, 2, \dots, N,$$

$$(2.21) \quad \bar{u}_n^c = C_h^\alpha \bar{u}_n + u_0 - \tilde{u}_{n-1} + \frac{h^\alpha}{\Gamma(1 + \alpha)} \sum_{j=1}^{n-1} w_{n,j}^\alpha f\left(t_{j-\frac{1}{2}}, \frac{\tilde{u}_{j-1} + \tilde{u}_j}{2}\right),$$

where

$$(2.22) \quad w_{n,j}^\alpha = \frac{\alpha}{h^\alpha} \int_{t_{j-1}}^{t_j} \frac{1}{(t_n - \tau)^{1-\alpha}} d\tau = (n - j + 1)^\alpha - (n - j)^\alpha.$$

To obtain (2.19), we used the following approximation,

$$\begin{aligned} ([t_n]I_{t_0}^\alpha A\tilde{u})(t_{n-1}) &= \frac{1}{\Gamma(\alpha)} \int_{t_0}^{t_{n-1}} \frac{A\tilde{u}(\tau)}{(t_n - \tau)^{1-\alpha}} d\tau = \frac{1}{\Gamma(\alpha)} \sum_{j=1}^{n-1} \int_{t_{j-1}}^{t_j} \frac{A\tilde{u}(\tau)}{(t_n - \tau)^{1-\alpha}} d\tau \\ &\approx \frac{A}{\Gamma(\alpha)} \sum_{j=1}^{n-1} \int_{t_{j-1}}^{t_j} \frac{\tilde{u}_j + \tilde{u}_{j+1}}{2} \frac{1}{(t_n - \tau)^{1-\alpha}} d\tau \\ &= \frac{Ah^\alpha}{2\Gamma(1 + \alpha)} \sum_{j=1}^{n-1} w_{n,j}^\alpha (\tilde{u}_{j-1} + \tilde{u}_j). \end{aligned}$$

The fractional integral $([t_n]I_{t_0}^\alpha f)(t_{n-1}, \tilde{u}(t_{n-1}))$ in (2.17) has been approximated similarly to obtain (2.21).

Remark 2.1. In the TS-I scheme and other numerical schemes we develop in the following, only $\tilde{u}_n, 1 \leq n \leq N$, is a numerical solution to (2.1), but $\bar{u}_n, 1 \leq n \leq N$, is not a numerical solution to (2.1). See also Remark 2.5 where we show that \bar{u} is not close to the exact solution for a similar splitting scheme.

For the time-splitting scheme TS-I, we have the following convergence theorem.

THEOREM 2.2 (convergence rate of the TS-I scheme). *Let $u(t)$ be the solution of (2.1) and $\tilde{u}_n, 0 \leq n \leq N$, be the solution of the time-splitting method (2.18)–(2.21). Suppose $h = T/N$ and $Ah^\alpha \neq \Gamma(1 + \alpha)I$.*

- *If $u \in C^2[0, T]$ and $f(t, u)$ satisfies the Lipschitz condition (2.2), then there exists a constant $C > 0$ independent of h such that*

$$(2.23) \quad |u(t_n) - \tilde{u}_n| \leq C(1 + |u'(0)|t_n^{-\alpha})h^{1+\alpha}, \quad 1 \leq n \leq N.$$

- *If $f \in C^2(G)$, then there exists a constant $C > 0$ independent of h such that*

$$(2.24) \quad |u(t_n) - \tilde{u}_n| \leq C(1 + t_n^{\alpha-1})h^{1+\alpha}, \quad 1 \leq n \leq N.$$

Remark 2.3 (regularity assumption). Equation (2.1) can have a smooth solution; see [9, 34, 39], etc. In fact, the assumption of $u(t) \in C^2[0, T]$ can be verified when f is only a function of t and $f \in C^2[0, T]$ with $f(0) = f'(0) = 0$ and $u_0 = 0$; see [34]. This can be readily checked since the solution u can be written as

$$u(t) = u_0 E_{\alpha,1}[At^\alpha] + \int_0^t (t - \tau)^{\alpha-1} E_{\alpha,\alpha}[A(t - \tau)^\alpha] f(\tau) d\tau,$$

where $E_{\alpha,\beta}[z] := \sum_{k=0}^\infty \frac{z^k}{\Gamma(\alpha k + \beta)}$ is the Mittag-Leffler-type function.

If $f \in C^2(G)$, the solution of (2.1) is not in $C^2[0, T]$ but is of the form

$$(2.25) \quad u(t) = \psi(t) + \sum_{\nu=1}^{\hat{\nu}} c_\nu t^{\nu\alpha},$$

where $\psi \in C^1[0, T]$ and $\hat{\nu} := [1/\alpha] - 1$; see [9, 11, 28].

Remark 2.4 (implementation). In practice, time-fractional differential equations may be of the form

$$({}^C D_0^\alpha u)(t) = g(t, u(t)), \quad t \in (0, T], \quad u(0) = u_0$$

instead of in the form (2.1). If a splitting scheme is used, one can decompose $g(t, u(t))$ as $Au(t) + f(t, u(t))$ so that A is stiff while $f(t, u(t))$ is less stiff; see, e.g., Examples 4.1 and 4.3 where the $g(t, u(t))$ are linear. To ensure the stability of the splitting schemes, one should follow the stability conditions in section 3, where linear stability for scalar equations is considered.

The term $-(I_{t_{n-1}}^\alpha A(\bar{u} - \tilde{u}))(t)$ is crucial to keep the convergence order of the splitting schemes. If this correction term is missing, we can only have a scheme of convergence order α , no matter what higher-order discretization methods are used. In other words, the splitting error is of order α . For example, if we apply the $(1 + \alpha)$ -order time discretization as in the splitting scheme (2.18)–(2.21) but drop the term $-(I_{t_{n-1}}^\alpha A(\bar{u} - \tilde{u}))(t_n)$, then we obtain the following time-splitting scheme (TS-II): for

$n = 1, 2, \dots, N,$

$$(2.26) \quad \bar{u}_n = \tilde{u}_{n-1}^c + \frac{Ah^\alpha}{\Gamma(1+\alpha)} \bar{u}_n,$$

$$(2.27) \quad \tilde{u}_{n-1}^c = \tilde{u}_{n-1} + \frac{Ah^\alpha}{2\Gamma(1+\alpha)} \sum_{j=1}^{n-1} w_{n,j}^\alpha (\tilde{u}_{j-1} + \tilde{u}_j), \quad \tilde{u}_0 = u_0,$$

$$(2.28) \quad \tilde{u}_n = \bar{u}_n^c + \frac{h^\alpha}{\Gamma(1+\alpha)} f(t_{n-1}, \tilde{u}_{n-1}),$$

$$(2.29) \quad \bar{u}_n^c = \bar{u}_n + u_0 - \tilde{u}_{n-1} + \frac{h^\alpha}{\Gamma(1+\alpha)} \sum_{j=1}^{n-1} w_{n,j}^\alpha f\left(t_{j-\frac{1}{2}}, \frac{\tilde{u}_{j-1} + \tilde{u}_j}{2}\right),$$

where $w_{n,j}^\alpha$ is from (2.22).

Remark 2.5 (splitting error). Consider the splitting method (2.7)–(2.10) without the term $-(I_{t_{n-1}}^\alpha A(\bar{u} - \tilde{u}))(t)$ in (2.10), which we present as follows:

$$\begin{aligned} \bar{v}(t) &= \tilde{v}_{n-1}^c + (I_{t_{n-1}}^\alpha A\bar{v})(t), \quad t_{n-1} < t \leq t_n, \\ \tilde{v}_{n-1}^c &= \tilde{v}(t_{n-1}) + ({}_{[t]}I_{t_0}^\alpha A\tilde{v})(t_{n-1}), \\ \tilde{v}(t) &= \bar{v}_n^c + (I_{t_0}^\alpha f)(t, \tilde{v}(t)), \quad t_{n-1} < t \leq t_n, \\ \bar{v}_n^c &= \bar{v}(t_n) - \tilde{v}(t_{n-1}) + v(t_0). \end{aligned}$$

This splitting method leads to the following integral representation

$$(2.30) \quad \tilde{v}(t) = v(t_0) + (I_{t_0}^\alpha f)(t, \tilde{v}(t)) + ({}_{[t_n]}I_{t_0}^\alpha A\tilde{v})(t_{n-1}) + (I_{t_{n-1}}^\alpha A\bar{v})(t_n).$$

From (2.5) and (2.30), we have, denoting $e(t) = \tilde{v}(t) - u(t)$,

$$\begin{aligned} e(t_n) &= (I_{t_0}^\alpha f)(t_n, \tilde{v}(t_n)) - (I_{t_0}^\alpha f)(t_n, u(t_n)) \\ &\quad + ({}_{[t_n]}I_{t_0}^\alpha A\tilde{v})(t_{n-1}) + (I_{t_{n-1}}^\alpha A\bar{v})(t_n) - (I_{t_0}^\alpha Au)(t_n). \end{aligned}$$

Since f satisfies the Lipschitz condition (2.2), we get

$$(2.31) \quad \begin{aligned} |e(t_n)| &\leq K(I_{t_0}^\alpha |e|)(t_n) + \|A\|({}_{[t_n]}I_{t_0}^\alpha |e|)(t_{n-1}) + (I_{t_{n-1}}^\alpha A|\bar{v} - u|)(t_n) \\ &\leq (K + \|A\|)(I_{t_0}^\alpha |e|)(t_n) + (I_{t_{n-1}}^\alpha A|\bar{v} - u|)(t_n). \end{aligned}$$

We assume that $\tilde{v}(t) = u(t)$ when $t \leq t_{n-1}$ and then have

$$\begin{aligned} \bar{v}(t) &= \tilde{v}(t_{n-1}) + ({}_{[t]}I_{t_0}^\alpha A\tilde{v})(t_{n-1}) + (I_{t_{n-1}}^\alpha A\bar{v})(t) \\ &= u(t_{n-1}) + ({}_{[t]}I_{t_0}^\alpha Au)(t_{n-1}) + (I_{t_{n-1}}^\alpha A\bar{v})(t). \end{aligned}$$

From (2.5), we can write

$$\begin{aligned} u(t) &= u(t_0) + (I_{t_0}^\alpha Au)(t) + (I_{t_0}^\alpha f)(t, u(t)) \\ &= u(t_{n-1}) - (I_{t_0}^\alpha Au)(t_{n-1}) - (I_{t_0}^\alpha f)(t_{n-1}, u(t_{n-1})) + (I_{t_0}^\alpha Au)(t) + (I_{t_0}^\alpha f)(t, u(t)). \end{aligned}$$

Thus we have $\bar{v} - u$ is of $O(1)$ since

$$\begin{aligned} \bar{v} - u &= ({}_{[t]}I_{t_0}^\alpha Au)(t_{n-1}) + (I_{t_{n-1}}^\alpha A\bar{v})(t) + (I_{t_0}^\alpha Au)(t_{n-1}) - (I_{t_0}^\alpha Au)(t) \\ &\quad + (I_{t_0}^\alpha f)(t_{n-1}, u(t_{n-1})) - (I_{t_0}^\alpha f)(t, u(t)) \\ &= (I_{t_{n-1}}^\alpha A(\bar{v} - u))(t) + (I_{t_0}^\alpha Au)(t_{n-1}) + (I_{t_0}^\alpha f)(t_{n-1}, u(t_{n-1})) - (I_{t_0}^\alpha f)(t, u(t)). \end{aligned}$$

Hence we have $(I_{t_{n-1}}^\alpha A|\bar{v} - u|)(t_n) \leq Ch^\alpha$. Then by the Gronwall-type inequality (see Lemma 6.19 in [10]), we have from (2.31) that $|e(t_n)| \leq Ch^\alpha E_{\alpha,1}[(K + \|A\|)t^\alpha]$.

We present the following convergence theorem for the TS-II scheme while we omit the proof as it is similar to that of Theorem 2.2.

THEOREM 2.6 (convergence order of the TS-II scheme). *Let $u(t)$ be the solution of (2.1) and $\tilde{u}_n, 0 \leq n \leq N$, be the solution of the time-splitting method (2.26)–(2.29). Suppose that either $u \in C^1[0, T]$ and $f(t, u)$ satisfies the Lipschitz condition (2.2), or $f \in C^2(G)$. Then for $h = T/N$, there exists a constant $C > 0$ independent of h such that*

$$(2.32) \quad \max_{1 \leq n \leq N} |u(t_n) - \tilde{u}_n| \leq Ch^\alpha.$$

2.2. A time-splitting scheme based on differential formulation. When $\alpha > 0$ is close to zero, the schemes in the previous subsection are of low order and close to 1 or 0. To obtain higher-order schemes when α is close to zero, we develop the following splitting scheme of convergence order $2 - \alpha$.

Instead of using the integral formulation (2.4), we use the differential formulation to derive our new splitting method. First, by the definitions of (1.2) and (2.3), we write (2.1) for $t \in (t_{n-1}, t_n]$, where $n \geq 1$ is an integer,

$$(2.33) \quad ({}^C D_{t_{n-1}}^\alpha u)(t) + ({}^C_{[t]} D_{t_0}^\alpha u)(t_{n-1}) = Au(t) + f(t, u(t)).$$

Applying the operator $(I_{t_{n-1}}^\alpha \cdot)(t)$ on both sides of (2.33), we have

$$(2.34) \quad u(t) - u(t_{n-1}) = -\frac{1}{\Gamma(\alpha)} \int_{t_{n-1}}^t \frac{({}^C_{[\tau]} D_{t_0}^\alpha u)(t_{n-1})}{(t - \tau)^{1-\alpha}} d\tau + (I_{t_{n-1}}^\alpha Au)(t) + (I_{t_{n-1}}^\alpha f)(t, u(t)).$$

To derive a splitting method, we assume that the solution over the time interval $[0, t_{n-1}]$ is known and we denote it by \tilde{u} . Denote \bar{u} such that

$$(2.35) \quad \bar{u}(t) = \tilde{u}(t_{n-1}) - \frac{1}{\Gamma(\alpha)} \int_{t_{n-1}}^t \frac{({}^C_{[\tau]} D_{t_0}^\alpha \tilde{u})(t_{n-1})}{(t - \tau)^{1-\alpha}} d\tau + (I_{t_{n-1}}^\alpha A\bar{u})(t),$$

where $t \in (t_{n-1}, t_n]$. We introduce “the initial value” of \bar{u} at t_{n-1} as

$$(2.36) \quad \bar{u}(t_{n-1}) = \tilde{u}(t_{n-1}).$$

By (2.34) and (2.35), it follows that

$$(2.37) \quad \tilde{u}(t) = \bar{u}(t) + \left(I_{t_{n-1}}^\alpha A(\tilde{u} - \bar{u}) \right) (t) + (I_{t_{n-1}}^\alpha f)(t, \tilde{u}(t)).$$

We introduce $\tilde{u}(t_{n-1}^+) = \bar{u}(t)$ as an initial condition to (2.37). Operating the Caputo derivative on both sides of (2.35) and (2.37), we have

$$(2.38) \quad \begin{aligned} ({}^C D_{t_{n-1}}^\alpha \bar{u})(t) &= -({}^C_{[t]} D_{t_0}^\alpha \tilde{u})(t_{n-1}) + A\bar{u}(t), \\ \bar{u}(t_{n-1}) &= \tilde{u}(t_{n-1}), \quad \tilde{u}(t_0) = u_0, \end{aligned}$$

$$(2.39) \quad \begin{aligned} ({}^C D_{t_{n-1}}^\alpha \tilde{u})(t) &= A(\tilde{u}(t) - \bar{u}(t)) + f(t, \tilde{u}(t)), \\ \tilde{u}(t_{n-1}^+) &= \bar{u}(t). \end{aligned}$$

Hence, we obtain the solution $\tilde{u}(t)$ for $t_{n-1} \leq t \leq t_n$, and by repeating the above process we can derive the solution over $(t_n, t_{n+1}]$. Here (2.38) and (2.39) have unique solutions when (2.1) has a unique solution as (2.38) is linear and (2.39) has the same form as (2.1).

We now consider time discretization of (2.38)–(2.39) over $t_{n-1} < t \leq t_n$. Taking $t = t_n$ and using the L1-discretization proposed in [34] for the fractional derivative in (2.39), we get

$$\begin{aligned} \frac{\hat{C}_h^\alpha \tilde{u}_n - \tilde{u}_{n-1}^c}{h} (I_{t_{n-1}}^{1-\alpha} 1)(t_n) &= -A\bar{u}_n + f(t_n, \tilde{u}_n), \\ \tilde{u}_{n-1}^c &= \bar{u}_n, \end{aligned}$$

where $\hat{C}_h^\alpha = I - h^\alpha \Gamma(2 - \alpha)A$ and $\tilde{u}_n \approx \tilde{u}(t_n)$, $\bar{u}_n \approx \bar{u}(t_n)$. We again take $t = t_n$ and use the L1-discretization to approximate fractional derivatives in (2.38) and have

$$\frac{\bar{u}_n - \tilde{u}_{n-1}}{h} (I_{t_{n-1}}^{1-\alpha} 1)(t_n) = - \sum_{k=1}^{n-1} \frac{\tilde{u}_k - \tilde{u}_{k-1}}{h} ({}_{[t_n]}I_{t_{k-1}}^{1-\alpha} 1)(t_k) + A\bar{u}_n.$$

Summing up all the discretizations for the different subequations, we have the following scheme:

$$(2.40) \quad \frac{\bar{u}_n - \bar{u}_{n-1}^c}{\Gamma(2 - \alpha)h^\alpha} = A\bar{u}_n, \quad \bar{u}_{n-1}^c = \tilde{u}_{n-1} - \sum_{k=1}^{n-1} w_{n,k}^{1-\alpha} (\tilde{u}_k - \tilde{u}_{k-1}),$$

$$(2.41) \quad \frac{\hat{C}_h^\alpha \tilde{u}_n - \tilde{u}_{n-1}^c}{\Gamma(2 - \alpha)h^\alpha} = f(t_n, \tilde{u}_n), \quad \tilde{u}_{n-1}^c = \hat{C}_h^\alpha \bar{u}_n,$$

where $w_{n,k+1}^{1-\alpha}$ is defined by (2.22). The time-splitting scheme (2.40)–(2.41) is fully implicit. To avoid nonlinear iterative solvers, we approximate the nonlinear term $f(t, u)$ by $f(t, u(t)) \approx f(t, u(s)) + f_u(t, u(s))(u(t) - u(s))$ (f_u is the first-order derivative with respect to u) when $t - s$ is small, and obtain the following time-splitting scheme (TS-III) with order $2 - \alpha$:

$$(2.42) \quad \frac{\bar{u}_n - \bar{u}_{n-1}^c}{\Gamma(2 - \alpha)h^\alpha} = A\bar{u}_n, \quad \bar{u}_{n-1}^c = \tilde{u}_{n-1} - \sum_{k=1}^{n-1} w_{n,k}^{1-\alpha} (\tilde{u}_k - \tilde{u}_{k-1}),$$

$$(2.43) \quad \begin{aligned} \tilde{C}_h^\alpha \tilde{u}_n &= \tilde{u}_{n-1}^c + \Gamma(2 - \alpha)h^\alpha \left(f(t_n, \tilde{u}_{n-1}) - \text{diag}[f_u(t_n, \tilde{u}_{n-1})] \tilde{u}_{n-1} \right), \\ \tilde{u}_{n-1}^c &= \tilde{C}_h^\alpha \bar{u}_n, \end{aligned}$$

where $\tilde{C}_h^\alpha = \hat{C}_h^\alpha - \Gamma(2 - \alpha)h^\alpha \text{diag}[f_u(t_n, \tilde{u}_{n-1})]$ and $\text{diag}[\cdot]$ denotes the diagonal matrix where the k th diagonal element is the k th element of a vector $k = 1, \dots, m$.

Based on Lemmas 4.1 and 4.2 and Theorem 4.1 in [34], we can prove the following theorem for the scheme (2.40)–(2.41) and the TS-III scheme.

THEOREM 2.7 (convergence order of the TS-III scheme). *Suppose that (2.1) has a solution $u \in C^2[0, T]$ and $u(0) = 0$, and $f(t, u)$ satisfies the Lipschitz condition (2.2) and has continuous second-order derivative with respect to the second argument. Let $\tilde{u}_n, 0 \leq n \leq N$, be the solution of the time-splitting scheme (2.40)–(2.41) or the TS-III scheme. Then for $h = T/N$ and $Ah^\alpha \Gamma(2 - \alpha) \neq I$, there exists a constant $C > 0$ independent of h such that*

$$(2.44) \quad \max_{1 \leq n \leq N} |u(t_n) - \tilde{u}_n| \leq Ch^{2-\alpha}.$$

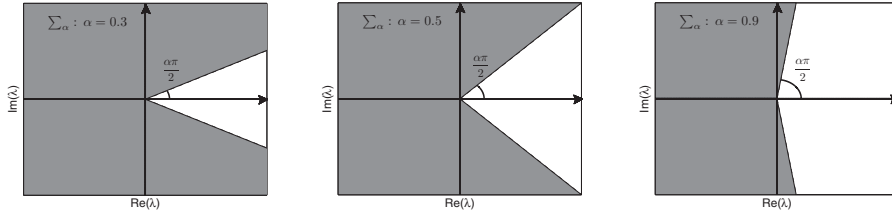


FIG. 1. Stability region of the test equation (3.1) for $0 < \alpha < 1$.

Remark 2.8. When $u(0) \neq 0$, it is natural to introduce $v(t) = u(t) - u(0)$ and a fractional differential equation that v satisfies. We then obtain the estimate (2.44) for v and thus the same estimate for u .

Remark 2.9. To show the performance of the TS-I and TS-III schemes when the exact solution is not smooth enough, we consider the following equation

$$(2.45) \quad ({}^C D_0^\alpha u)(t) = f(t), \quad t \in (0, T], \quad u(0) = u_0,$$

where $f(t) = \frac{\Gamma(p+\alpha+1)}{\Gamma(p+1)} t^p$, $p + \alpha \geq 0$, and the exact solution is $u(t) = t^{p+\alpha}$. For the TS-I scheme, there is a number $\alpha_0 \approx 0.4$ (obtained numerically) such that if $p \geq \max\{0, \alpha - \alpha_0\}$, the convergence order of the TS-I scheme at $t = T$ is $1 + \alpha$, while if $0 \leq p < \alpha - \alpha_0$, the order is $\max\{1, p + \alpha\}$. The TS-III scheme is exact if $p + \alpha = 1$ and for $p + \alpha < 1$, its convergence order at $t = T$ is $p + 1$; for $p + \alpha > 1$, the order is $2 - \alpha$. When $p + \alpha = 0$, then $u(t) = 1$ and the convergence order of the TS-III scheme at $t = T$ is $p + 1 = 1 - \alpha$.

3. Linear stability of time-splitting schemes. In this section, we discuss the linear stability of all proposed time-splitting schemes for the scalar equation (1.1).

We recall the definition of stability for the linear equation (1.1) and numerical methods.

THEOREM 3.1 (see [29, 30]). *Let $\alpha > 0$. The steady state $u = 0$ of (1.1) is stable if and only if $(\lambda + \sigma) \in \sum_\alpha$, where $\sum_\alpha = \{s \in \mathbb{C} : |\arg(s)| > \frac{\alpha\pi}{2}\}$.*

DEFINITION 3.2. *A numerical method is said to be $A(\frac{\alpha\pi}{2})$ -stable if its stability region for (3.1) contains the whole sector \sum_α .*

3.1. Stability of the TS-I and TS-II schemes. We first consider the stability of the TS-I and TS-II schemes for the following test equation ($\sigma = 0$ in (1.1)) where we can draw the stability region (see Figure 1):

$$(3.1) \quad ({}^C D_0^\alpha u)(t) = \lambda u(t), \quad t \geq 0, \quad \lambda \in \mathbb{C}.$$

We need the following theorem to determine stability regions of the TS-I and TS-II schemes.

THEOREM 3.3 (see [17, 19, 31]). *Let $\alpha > 0$. Assume that the sequence $\{g_n\}$ is convergent and that the quadrature weights w_n ($n \geq 1$) satisfy*

$$(3.2) \quad w_n = \frac{n^{\alpha-1}}{\Gamma(\alpha+1)} + v_n, \quad \sum_{n=1}^{\infty} |v_n| < \infty,$$

then the stability region of the convolution quadrature $y_n = g_n + z \sum_{j=0}^n w_{n-j} y_j$ is

$$\sum_\alpha^{Num} = \{z \in \mathbb{C} : 1 - zw^\alpha(\xi) \neq 0 : |\xi| \leq 1\}, \quad w^\alpha(\xi) = \sum_{n=0}^{\infty} w_n \xi^n,$$

where $z = \lambda h^\alpha$ or z is some function of λh^α .

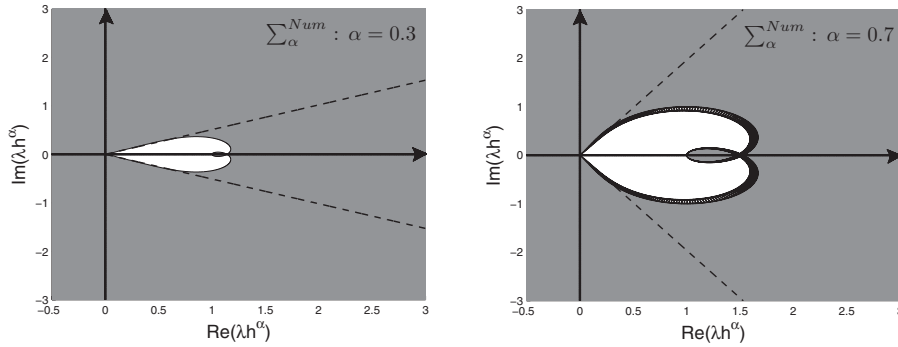


FIG. 2. Stability region of the TS-I scheme (shaded) for the test equation (3.1); left: $\alpha = 0.3$, right: $\alpha = 0.7$.

Stability analysis of the TS-I scheme. Applying the TS-I scheme (2.18)–(2.21) to the test equation (3.1), i.e., applying (2.18)–(2.21) with $f(t, u) = 0$, we get

$$(3.3) \quad \tilde{u}_n = \left(1 - \frac{\lambda h^\alpha}{2\Gamma(1+\alpha)} [(n+1)^\alpha - n^\alpha] \right) u_0 + \lambda h^\alpha \sum_{j=0}^n w_{n-j}^{(I)} \tilde{u}_j,$$

where $w_0^{(I)} = \frac{1}{\Gamma(1+\alpha)}$, $w_1^{(I)} = \frac{2^\alpha - 1^\alpha}{2\Gamma(1+\alpha)}$, $w_n^{(I)} = \frac{(n+1)^\alpha - (n-1)^\alpha}{2\Gamma(1+\alpha)}$. Then by Theorem 3.3, the stability region of the TS-I scheme is

$$\Sigma_\alpha^{Num} = \mathbb{C} \setminus \left\{ \frac{1}{w^I(\xi)} : |\xi| \leq 1 \right\}, \text{ where } w^I(\xi) = \sum_{n=0}^\infty w_n^{(I)} \xi^n.$$

In Figure 2, we plot the stability regions of the TS-I scheme for $\alpha = 0.3$ and $\alpha = 0.7$, where we take $n = 10^5$ in (3.3), as the function $w^I(\xi) = \sum_{n=0}^\infty w_n^{(I)} \xi^n$ is not explicitly known. We can see that the TS-I scheme is $A(\frac{\alpha\pi}{2})$ -stable as $\Sigma_\alpha \subset \Sigma_\alpha^{Num}$ for $\alpha = 0.3, 0.7$.

Stability analysis of the TS-II scheme. The TS-II scheme (2.26)–(2.29) for the test equation (3.1) ($f(t, u) = 0$ in (2.1)) reads

$$(3.4) \quad \tilde{u}_n = u_0 + \frac{\lambda h^\alpha}{\Gamma(1+\alpha)} \bar{\tilde{u}}_n + \frac{\lambda h^\alpha}{2\Gamma(1+\alpha)} \sum_{j=1}^{n-1} w_j^\alpha (\tilde{u}_{j-1} + \tilde{u}_j).$$

Substituting (2.26) into (3.4), we have

$$\tilde{u}_n = \left(1 - \frac{\lambda h^\alpha}{2(\Gamma(1+\alpha) - \lambda h^\alpha)} [(n+1)^\alpha - n^\alpha] \right) u_0 + \frac{\lambda h^\alpha}{\Gamma(1+\alpha) - \lambda h^\alpha} \sum_{j=0}^n w_{n-j}^{(II)} \tilde{u}_j,$$

where $w_0^{(II)} = 0$, $w_1^{(II)} = \frac{2^\alpha - 1^\alpha}{2} + 1$, $w_n^{(II)} = \frac{(n+1)^\alpha - (n-1)^\alpha}{2}$. Then, by Theorem 3.3, the stability region of the TS-II scheme is

$$\Sigma_\alpha^{Num} = \mathbb{C} \setminus \left\{ \frac{\Gamma(1+\alpha)}{1 + w^{II}(\xi)} : |\xi| \leq 1 \right\}, \text{ where } w^{II}(\xi) = \sum_{n=0}^\infty w_n^{(II)} \xi^n.$$

It can be readily proved that the scheme is stable if $Re(\lambda) < 0$. In Figure 3, we plot the stability region of the TS-II scheme numerically (with $n = 2 \times 10^5$). The

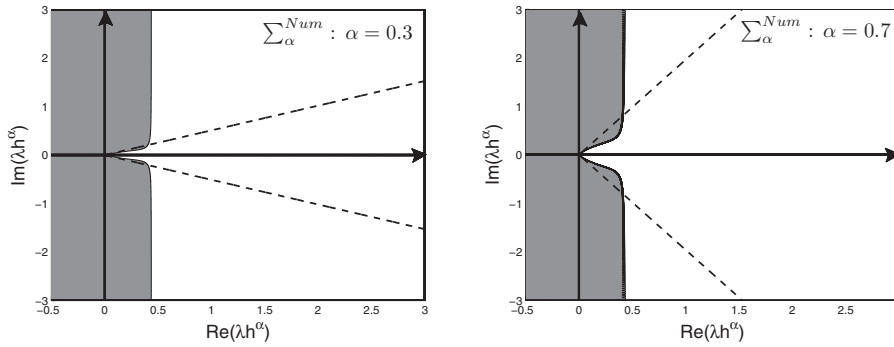


FIG. 3. Stability region (shaded) of the TS-II scheme for the test equation (3.1); left: $\alpha = 0.3$, right: $\alpha = 0.7$.

TS-II scheme is not $A(\frac{\alpha\pi}{2})$ -stable as Σ_α is not a subset of Σ_α^{Num} . When $Re(\lambda) > 0$, we will need a small step size h to ensure the stability of the TS-II scheme.

Now we consider the test equation (1.1) with $\sigma \neq 0$. From the TS-I scheme (2.18)–(2.21), we get

$$(3.5) \quad \begin{aligned} \tilde{u}_n = & \left(1 - \frac{(\lambda + \sigma)h^\alpha}{2\Gamma(1 + \alpha)} [(n + 1)^\alpha - n^\alpha] \right) u_0 \\ & + (\lambda + \sigma)h^\alpha \sum_{j=0}^{n-1} w_{n-j}^{(I)} \tilde{u}_j + \frac{\sigma h^\alpha \tilde{u}_{n-1}}{\Gamma(1 + \alpha)} + \frac{\lambda h^\alpha \tilde{u}_n}{\Gamma(1 + \alpha)}, \end{aligned}$$

where $w_j^{(I)}$ is from (3.3). By letting the roots of the characteristic polynomial of (3.5) be less than one, we obtain that the TS-I scheme is asymptotically stable, that is, $\lim_{n \rightarrow \infty} \tilde{u}_n = 0$ for the fixed step size h ($T \rightarrow \infty$) if

$$2\Gamma(\alpha + 1)\text{Re}(\sigma + \lambda) \leq (|\lambda|^2 - |\sigma|^2)h^\alpha.$$

Since the TS-II scheme is only of order α and is of little use in practice, we will not discuss the stability condition here.

3.2. Stability analysis of the TS-III scheme. We need the following conclusion to determine the stability region of the TS-III scheme. We omit the proof for this theorem as it is a straightforward application of Propositions 5 and 6 in [14] or the results in [31].

THEOREM 3.4. *Let $\alpha > 0$. If the quadrature weights w_n ($n \geq 0$) are defined by*

$$(3.6) \quad w_0 = 1, \quad w_n = (n + 1)^{1-\alpha} + (n - 1)^{1-\alpha} - 2n^{1-\alpha}, \quad (n \geq 1),$$

and $b_n = n^{1-\alpha} - (n - 1)^{1-\alpha}$, then the stability region for the convolution quadrature $\sum_{j=0}^{n-1} w_{n-j} y_j - b_{n+1} y_0 = (\lambda + \sigma)h^\alpha \Gamma(2 - \alpha) y_n$ is

$$\Sigma_\alpha^{Num} = \{z \in \mathbb{C} \mid w(\xi) - z\Gamma(2 - \alpha) \neq 0 : |\xi| \leq 1\}, \quad w(\xi) = \sum_{n=0}^{\infty} w_n \xi^n.$$

The TS-III scheme (2.42)–(2.43) for the test equation (1.1) is

$$(3.7) \quad \sum_{j=0}^n w_{n-j}^{(III)} \tilde{u}_j = \Gamma(2 - \alpha)(\lambda + \sigma)h^\alpha \tilde{u}_n$$

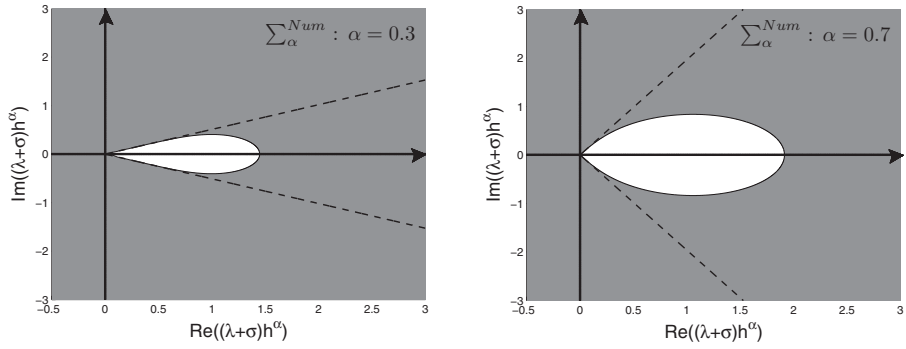


FIG. 4. Stability region of the TS-III scheme (shaded) for the test equation (1.1); left: $\alpha = 0.3$, right: $\alpha = 0.7$.

and $w_j^{(III)}$ is from (3.6). By Theorem 3.4, the stability region of the TS-III scheme is

$$(\lambda + \sigma)h^\alpha \in \Sigma_\alpha^{Num} = \mathbb{C} \setminus \left\{ \frac{w^{III}(\xi)}{\Gamma(2 - \alpha)} : |\xi| \leq 1 \right\}, \text{ where } w^{III}(\xi) = \sum_{n=0}^{\infty} w_n^{(III)} \xi^n.$$

The TS-III scheme is $A(\frac{\alpha\pi}{2})$ -stable. In Figure 4, we plot the stability region numerically (with $n = 10^5$).

4. Numerical examples. We denote by u_n^h a numerical solution of the time-splitting schemes with a time step size h at $t_n = nh$, and we measure the errors in the following sense:

$$E_\infty^r(h) = \frac{\max_{1 \leq n \leq N} |u_n^{\text{ref}} - u_n^h|}{\max_{1 \leq n \leq N} |u_n^{\text{ref}}|} \text{ or } E_N^r(h) = \frac{|u_N^{\text{ref}} - u_N^h|}{|u_N^{\text{ref}}|},$$

where $t_N = Nh = T$. When u_n^h is a vector, $|\cdot|$ denotes the infinity norm of vectors. If an exact solution is available, we take u_n^{ref} as the exact solution $u(t_n)$; otherwise, we calculate u_n with the step size $h_0 = 2^{-15}$ as the reference solution.

We will test convergence orders of the proposed TS-I, TS-III, and TS-II schemes for linear systems in Example 4.1 with both smooth and nonsmooth solutions. We also use the TS-I and TS-III schemes to solve the time-fractional reaction-diffusion equation in Example 4.2. In Example 4.3, we use the TS-I scheme but with substepping for a stiff linear system to show the flexibility of a time-splitting method. In the first two examples, we also compare our schemes with the predictor-corrector scheme (4.1)–(4.2) from [8]:

$$(4.1) \quad u_{n+1}^p = u_0 + \frac{h^\alpha}{\Gamma(\alpha + 1)} \sum_{j=0}^n w_{nj}^\alpha f(t_j, u_j),$$

$$(4.2) \quad u_{n+1} = u_0 + \frac{h^\alpha}{\Gamma(\alpha + 2)} f(t_{n+1}, u_{n+1}^p) + \frac{h^\alpha}{\Gamma(\alpha + 2)} \sum_{j=0}^n a_{j,n+1} f(t_j, u_j),$$

where w_{nj}^α is the same as (2.22) and

$$a_{j,n+1} = \begin{cases} n^{\alpha+1} - (n - \alpha)(n + 1)^\alpha & \text{if } j = 0, \\ (n - j + 2)^{\alpha+1} + (n - j)^{\alpha+1} - 2(n - j + 1)^{\alpha+1} & \text{if } 1 \leq j \leq n. \end{cases}$$

Example 4.1 (linear time-fractional differential equation).

$$(4.3) \quad \begin{aligned} ({}^C D_0^\alpha u)(t) &= (A + B)u(t) + f(t), t \in (0, T], \\ u(0) &= u_0. \end{aligned}$$

Case 1. Smooth solution. Take $u_0 = (0, 0, 0)^\top$ and

$$(4.4) \quad A = \begin{pmatrix} -1000 & 0 & 1 \\ -0.5 & -0.8 & -0.2 \\ 1 & 0 & -1 \end{pmatrix}, \quad B = \begin{pmatrix} -0.6 & 0 & 0.2 \\ -0.1 & -0.2 & 0 \\ 0 & -0.5 & -0.8 \end{pmatrix},$$

and

$$(4.5) \quad f(t) = \begin{pmatrix} a_1 \Gamma_1 t^{m_1 - \alpha} + a_2 \Gamma_1 t^{m_2 - \alpha} \\ a_2 \Gamma_2 t^{m_2 - \alpha} + a_3 \Gamma_2 t^{m_3 - \alpha} \\ a_3 \Gamma_3 t^{m_3 - \alpha} + a_1 \Gamma_3 t^{m_1 - \alpha} \end{pmatrix} - (A + B) \begin{pmatrix} a_1 t^{m_1} + a_2 t^{m_2} \\ a_2 t^{m_2} + a_3 t^{m_3} \\ a_3 t^{m_3} + a_1 t^{m_1} \end{pmatrix},$$

where $\Gamma_i = \frac{\Gamma(m_i + 1)}{\Gamma(m_i + 1 - \alpha)}$, $i = 1, 2, 3$, and the exact solution is

$$(4.6) \quad u(t) = (a_1 t^{m_1} + a_2 t^{m_2}, a_2 t^{m_2} + a_3 t^{m_3}, a_3 t^{m_3} + a_1 t^{m_1})^\top.$$

Here, we take $m_1 = 5/2$, $m_2 = 3$, $m_3 = 7/3$, $a_1 = 0.5$, $a_2 = 0.8$, $a_3 = 1$.

Case 2. Nonsmooth solution. Let $u_0 = (1, 3)^\top$ and

$$(4.7) \quad A = \begin{pmatrix} 0.35 & 0 \\ 0.1 & 0.2 \end{pmatrix}, \quad B = \begin{pmatrix} 0.15 & 0.5 \\ 0.4 & 0.3 \end{pmatrix}, \quad f(t) = 0,$$

then the exact solution is

$$u_1(t) = -\frac{1}{2} + \frac{3}{2} E_\alpha[t^\alpha], \quad u_2(t) = \frac{3}{2}(1 + E_\alpha[t^\alpha]).$$

In Case 1, the exact solution (4.6) has bounded first- and second-order derivatives and thus the convergence order of the TS-I scheme (2.18)–(2.21) is $1 + \alpha$ according to Theorem 2.2 and Remark 5.5, and the convergence order of the TS-III scheme (2.42)–(2.43) is $2 - \alpha$ by Theorem 2.7.

We test the numerical performance of the TS-I scheme and the TS-III scheme in Case 1. In Table 1 and Figure 5, we solve this linear system up to $T = 64$; the TS-I scheme is of order $1 + \alpha$ and the TS-III schemes is of order $2 - \alpha$, as expected from Theorem 2.2, Remark 5.5 and Theorem 2.7. However, the computational time of the TS-I scheme is larger than that of the TS-III scheme. The reason is that we need to calculate two convolutions in TS-I, including a convolution with respect to the nonlinear term $f(t, u)$, while we calculate just one convolution in TS-III in every step, which has the main impact on the computational complexity. To show the difference in computational time, we illustrate the CPU time of running both the TS-I scheme and the TS-III scheme for Case 1 in Table 1.

With the TS-I scheme and the TS-III scheme, we solve the stiff time-fractional differential equation up to $T = 64$. In contrast, the predictor-corrector scheme (4.1)–(4.2) blows up very quickly even at $T = 1/32$ and with very small time step sizes (numerical results are not presented).

In Case 2, we have a nonsmooth solution to (4.3) with (4.7): the exact solution does not have bounded first- and second-order derivatives at $t = 0$. The schemes TS-I

TABLE 1

Convergence rate of the time-splitting scheme *TS-I* (2.18)–(2.21) and *TS-III* (2.42)–(2.43) for system (4.3) with the coefficients (4.4) and (4.5) up to $T = 64$ (Case 1).

	h	$\alpha = 0.1$		$\alpha = 0.5$		$\alpha = 0.9$		CPU Time
		$E_\infty^r(h)$	Order	$E_\infty^r(h)$	Order	$E_\infty^r(h)$	Order	
TS-I	2^{-7}	7.75e-04	1.10	5.40e-05	1.50	3.14e-06	1.91	18.2
	2^{-8}	3.61e-04	1.10	1.91e-05	1.50	8.38e-07	1.90	72.4
	2^{-9}	1.69e-04	1.10	6.74e-06	1.50	2.24e-07	1.90	288.0
	2^{-10}	7.87e-05	*	2.38e-06	*	5.98e-08	*	1152.0
TS-III	2^{-7}	1.48e-08	1.85	4.10e-07	1.50	3.43e-06	1.10	8.9
	2^{-8}	4.11e-09	1.86	1.45e-07	1.50	1.60e-06	1.10	34.0
	2^{-9}	1.14e-09	1.86	5.13e-08	1.50	7.47e-07	1.10	133.6
	2^{-10}	3.13e-10	*	1.82e-08	*	3.49e-07	*	529.1

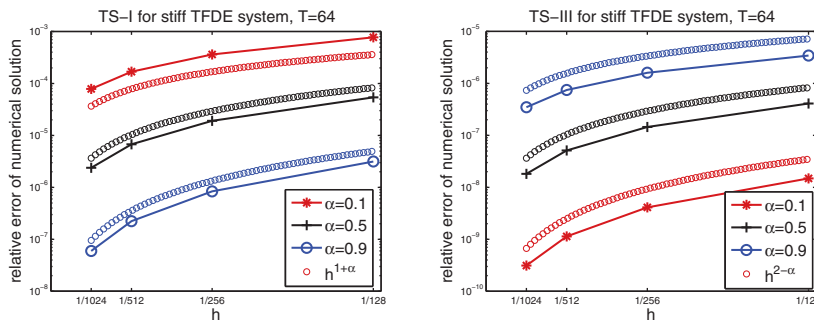


FIG. 5. Comparison of the convergence order between the schemes *TS-I*, *TS-III* for the stiff time-fractional differential equation (4.3) with coefficients (4.4) and (4.5) (Example 1, Case 1). Solid lines are the relative error in the maximum norm of numerical solutions, versus the step size h , corresponding to $\alpha = 0.1, 0.5, 0.9$.

and *TS-II* are still of order $1 + \alpha$ and α , respectively (see Table 2), which verify the results in Theorems 2.2 and 2.6. The convergence order of the *TS-I* scheme is also in agreement with our observations for a simple problem in Remark 2.9. In Table 2, we also observe that the predictor-corrector scheme is of order $1 + \alpha$ while the scheme *TS-III* is only of order $1 - \alpha$. The low order of the *TS-III* scheme for this case is due to the nonsmooth exact solution with the nonzero initial value, which is in agreement with our observations in Remarks 2.9 and 2.3 when the initial condition is not zero.

Example 4.2 (time fractional reaction-diffusion equation).

$$(4.8) \quad ({}^C D_0^\alpha u)(x, t) = u_{xx} + u(1 - u)(1 + u), \quad (x, t) \in (-\pi, \pi) \times (0, T],$$

$$(4.9) \quad u(x, 0) = \sin(x), \quad x \in (-\pi, \pi),$$

$$(4.10) \quad u(-\pi, t) = u(\pi, t) = 0, \quad t \in [0, T].$$

We adopt the Fourier collocation method with M points ($M = 512$ in the numerical test) in physical space and obtain the following time-fractional differential equation

$$(4.11) \quad ({}^C D_0^\alpha \vec{u})(t) = D^2 \vec{u}(t) + \vec{u}(t) \circ (1 - \vec{u}(t)) \circ (1 + \vec{u}(t)), \quad t \in (0, T],$$

where “ D ” is the Fourier spectral differential matrix, “ \circ ” denotes the Hadamard

TABLE 2

Convergence rate of the time-splitting scheme: TS-I (2.18)–(2.21), TS-II (2.26)–(2.29), TS-III (2.42)–(2.43) for nonstiff equation (4.3) with (4.7) (Example 1, Case 2) up to $T = 1$ and a comparison with the predictor-corrector scheme (4.1)–(4.2).

	h	$\alpha = 0.1$		$\alpha = 0.5$		$\alpha = 0.9$	
		$E_N^r(h)$	Order	$E_N^r(h)$	Order	$E_N^r(h)$	Order
TS-I	2^{-7}	6.04e-02	1.10	1.12e-03	1.48	2.88e-05	1.84
	2^{-8}	2.82e-02	1.10	4.02e-04	1.49	8.03e-06	1.84
	2^{-9}	1.32e-02	1.10	1.43e-04	1.49	2.24e-06	1.83
	2^{-10}	6.15e-03	1.10	5.10e-05	1.49	6.28e-07	1.84
	2^{-11}	2.87e-03	*	1.81e-05	*	1.76e-07	*
TS-II	2^{-7}	7.05e-01	0.02	2.26e-02	0.43	1.52e-03	0.84
	2^{-8}	6.95e-01	0.03	1.68e-02	0.47	8.48e-04	0.87
	2^{-9}	6.79e-01	0.06	1.21e-02	0.49	4.64e-04	0.88
	2^{-10}	6.51e-01	0.08	8.67e-03	0.49	2.52e-04	0.89
	2^{-11}	6.17e-01	*	6.16e-03	*	1.35e-04	*
TS-III	2^{-7}	1.13e-02	0.85	1.11e-01	0.48	6.67e-01	0.10
	2^{-8}	6.27e-03	0.86	8.00e-02	0.48	6.25e-01	0.10
	2^{-9}	3.46e-03	0.86	5.72e-02	0.49	5.84e-01	0.10
	2^{-10}	1.90e-03	0.87	4.07e-02	0.49	5.46e-01	0.10
	2^{-11}	1.04e-03	*	2.89e-02	*	5.09e-01	*
P-C	2^{-7}	5.11e-02	1.05	1.09e-03	1.48	3.83e-05	1.86
	2^{-8}	2.46e-02	1.08	3.89e-04	1.49	1.06e-05	1.87
	2^{-9}	1.17e-02	1.09	1.39e-04	1.49	2.90e-06	1.87
	2^{-10}	5.48e-03	1.09	4.93e-05	1.49	7.93e-07	1.87
	2^{-11}	2.57e-03	*	1.75e-05	*	2.17e-07	*

TABLE 3

Convergence rate of the time-splitting scheme (upper: TS-I (2.18)–(2.21); lower: TS-III (2.42)–(2.43) for nonlinear time-fractional reaction-diffusion equation (4.8)–(4.10) up to $T = 1$ with $M = 512$ Fourier collocation points.

	h	$\alpha = 0.1$		$\alpha = 0.5$		$\alpha = 0.9$	
		$E_N^r(h)$	Order	$E_N^r(h)$	Order	$E_N^r(h)$	Order
TS-I	2^{-7}	5.09e-05	1.05	2.36e-05	1.45	3.35e-06	1.93
	2^{-8}	2.45e-05	1.06	8.63e-06	1.46	8.81e-07	1.92
	2^{-9}	1.18e-05	1.07	3.14e-06	1.47	2.33e-07	1.91
	2^{-10}	5.60e-06	1.10	1.13e-06	1.49	6.20e-08	1.91
TS-III	2^{-5}	1.72e-04	1.03	7.89e-04	1.05	1.53e-03	1.01
	2^{-6}	8.42e-05	1.03	3.82e-04	1.04	7.59e-04	1.02
	2^{-7}	4.12e-05	1.04	1.86e-04	1.04	3.74e-04	1.03
	2^{-8}	2.00e-05	1.06	9.04e-05	1.06	1.83e-04	1.05

product of vectors, and

$$\vec{u}(t) \approx (u(x_1, t), u(x_2, t), \dots, u(x_M, t))^T, \quad x_j = -\pi + \frac{2\pi j}{M}, \quad j = 1, 2, \dots, M.$$

Then we apply our time-splitting schemes and the predictor-corrector scheme to solving (4.11) in time.

In Table 3, we observe that the TS-I scheme is of order $1 + \alpha$ while the TS-III scheme is of order 1. We also solve (4.11) by the predictor-corrector scheme and observe in Table 4 that the predictor-corrector scheme blows up very quickly ($T = 1/32$) when $\alpha = 0.1, 0.5$ even with very small step sizes. When $\alpha = 0.9$, the predictor-corrector scheme requires small time step sizes for the same level of accuracy,

TABLE 4

Convergence rate of the predictor-corrector scheme for nonlinear time-fractional reaction-diffusion equation (4.8)–(4.10) using $M = 512$ Fourier collocation points.

h	$\alpha = 0.1, T = 1/32$	$\alpha = 0.5, T = 1/32$	$\alpha = 0.9, T = 1$	
	$E_N^r(h)$	$E_N^r(h)$	$E_N^r(h)$	Order
2^{-9}	Calculation failed	Calculation failed	1.33e-04	1.86
2^{-10}	Calculation failed	Calculation failed	3.67e-05	1.87
2^{-11}	Calculation failed	Calculation failed	1.00e-05	1.87
2^{-12}	Calculation failed	Calculation failed	2.74e-06	1.88

compared to our time splitting schemes. In this case, the TS-III scheme is of first order, not of order $2 - \alpha$.

This can be explained by the fact that the solutions do not have bounded second-order derivatives as required in Theorem 2.7. The first-order convergence in time suggests that the solutions have bounded first-order derivatives, which should be carefully analyzed in theory but we do not consider in this paper.

Example 4.3 (substepping in the time-splitting scheme TS-I). Consider a substepping in the TS-I scheme for the time-fractional differential equation (4.3) with coefficients

$$(4.12) \quad A = \begin{pmatrix} -10000 & 0 \\ 0 & 0.001 \end{pmatrix}, \quad B = \begin{pmatrix} 10 & 0 \\ 0 & 8 \end{pmatrix}, \quad f(t) = 0, \quad u_0 = (1, 1)^\top.$$

We apply the TS-I scheme (2.18)–(2.21) to the above equation while we also apply a substepping in time: for $n = 1, 2, \dots, N$,

$$(4.13) \quad \bar{u}_n = \tilde{u}_{n-1}^c + \frac{Ah^\alpha}{\Gamma(1 + \alpha)} \bar{u}_n,$$

$$(4.14) \quad \tilde{u}_{n-1}^c = \tilde{u}_{n-1} + \frac{Ah^\alpha}{2\Gamma(1 + \alpha)} \sum_{j=1}^{n-1} w_{n,j}^\alpha (\tilde{u}_{j-1} + \tilde{u}_j), \quad \tilde{u}_0 = u_0,$$

$$(4.15) \quad C_h^\alpha \tilde{u}_{n_m} = \bar{u}_{n_m}^c + \frac{Bh_s^\alpha \tilde{u}_{n_m-1}}{\Gamma(1 + \alpha)}, \quad n_m = m(n - 1) + 1, \dots, mn, \quad m = h/h_s,$$

$$(4.16) \quad \bar{u}_{n_m}^c = C_h^\alpha \bar{u}_n + u_0 - \tilde{u}_{n-1} + \frac{Bh_s^\alpha}{\Gamma(1 + \alpha)} \sum_{j=1}^{n_m-1} w_{n_m,j}^\alpha \frac{\tilde{u}_{j-1} + \tilde{u}_j}{2},$$

$$(4.17) \quad \tilde{u}_n = \tilde{u}_{mn},$$

where $h_s \leq h$ is the substepping time step size; $C_h^\alpha = I - \frac{Ah^\alpha}{\Gamma(1 + \alpha)}$, and $w_{n,j}^\alpha = (n - j + 1)^\alpha - (n - j)^\alpha$. We note that taking $h_s = h$ leads to the TS-I scheme (2.18)–(2.21). We compare numerical results from (4.13)–(4.17) with $h_s < h$ and those obtained by the TS-I scheme with a single time step size ($h_s = h$). In Table 5, we observe that when taking $h_s = h = 2^{-3}, 2^{-4}, 2^{-5}, 2^{-6}$, the TS-I scheme does not work for this stiff equation. We need to take much smaller step sizes $h_s = h = 2^{-10}, 2^{-11}, 2^{-12}, 2^{-13}$. With a substepping (4.15)–(4.16), we can compute this stiff equation with satisfactory accuracy at $T = 1$. Compared to taking $h_s = h$ in the TS-I scheme, the TS-I scheme with substepping (4.13)–(4.17) takes only half the computational time to achieve the same level of accuracy.

5. Proofs. In this section, we prove Theorem 2.2. We will study error estimates of our quadrature rules and then provide a proof of Theorem 2.2.

TABLE 5

Convergence rate of the TS-I scheme (2.18)–(2.21) for (4.3) with coefficients (4.12). Left: identical large step size; middle: different step sizes for different subequations; right: identical small step size. $\alpha = 0.5, T = 1$.

h	$E_N^r(h)$	h/h_s	$E_N^r(h)$	Order	Time (s.)	h	$E_N^r(h)$	Order	Time (s.)
2^{-3}	1.0000e-00	$2^{-3}/2^{-10}$	7.64e-01	0.90	0.35	2^{-10}	7.62e-01	0.89	0.71
2^{-4}	1.0000e-00	$2^{-4}/2^{-11}$	4.10e-01	1.29	1.40	2^{-11}	4.12e-01	1.27	2.79
2^{-5}	1.0000e-00	$2^{-5}/2^{-12}$	1.68e-01	1.54	5.50	2^{-12}	1.70e-01	1.52	11.0
2^{-6}	1.0000e-00	$2^{-6}/2^{-13}$	5.79e-02	1.91	21.5	2^{-13}	5.95e-02	1.89	42.5

5.1. Error estimate for quadrature rules. We define the errors of two quadrature rules which we use in the scheme TS-I,

$$\begin{aligned}
 R_n^{(1)} &= (I_{t_0}^\alpha g)(t_n) - \sum_{k=1}^{n-1} \frac{g(t_{k-1}) + g(t_k)}{2} \left({}_{[t_n]}I_{t_{k-1}}^\alpha 1 \right) (t_k) - g(t_{n-1})(I_{t_{n-1}}^\alpha 1)(t_n) \\
 (5.1) \quad &= \sum_{k=1}^{n-1} \left({}_{[t_n]}I_{t_{k-1}}^\alpha \left(g - \frac{g(t_{k-1}) + g(t_k)}{2} \right) \right) (t_k) + (I_{t_{n-1}}^\alpha (g - g(t_{n-1}))) (t_n),
 \end{aligned}$$

and

$$\begin{aligned}
 R_n^{(2)} &= (I_{t_0}^\alpha g)(t_n) - \sum_{k=1}^{n-1} \frac{g(t_{k-1}) + g(t_k)}{2} \left({}_{[t_n]}I_{t_{k-1}}^\alpha 1 \right) (t_k) - g(t_n)(I_{t_{n-1}}^\alpha 1)(t_n) \\
 (5.2) \quad &= \sum_{k=1}^{n-1} \left({}_{[t_n]}I_{t_{k-1}}^\alpha \left(g - \frac{g(t_{k-1}) + g(t_k)}{2} \right) \right) (t_k) + (I_{t_{n-1}}^\alpha (g - g(t_n))) (t_n).
 \end{aligned}$$

For our quadrature rule, we reach the following conclusions.

LEMMA 5.1. Suppose $g \in C^1[0, T]$ and $g'(t)$ fulfills a Hölder continuous condition

$$(5.3) \quad |g'(t_1) - g'(t_2)| \leq L|t_1 - t_2|^\beta, \quad 0 \leq \beta \leq 1, \quad \forall t_1, t_2 \in [0, T].$$

Then there exists a constant C independent of the step size h , such that for $1 \leq n \leq N$

$$(5.4) \quad |R_n^{(1)}| \leq Ch^{1+\min(\alpha, \beta)}, \quad |R_n^{(2)}| \leq Ch^{1+\min(\alpha, \beta)}.$$

LEMMA 5.2. For $g(t) = t^p, 0 \leq p \leq 1$, there exists a constant $C_{\alpha, p}$, which depends on α and p but is independent of the step size h , such that for $1 \leq n \leq N$

$$(5.5) \quad |R_n^{(1)}| \leq C_{\alpha, p} \max\{h^2 t_n^{\alpha+p-2}, h^{1+\alpha} t_n^{p-1}\},$$

$$(5.6) \quad |R_n^{(2)}| \leq C_{\alpha, p} \max\{h^2 t_n^{\alpha+p-2}, h^{1+\alpha} t_n^{p-1}\}.$$

Proof of Lemma 5.1. By the Taylor expansions, for $t \in [t_{k-1}, t_k]$, we have

$$\begin{aligned}
 g(t_{k-1}) &= g(t) + g'(t)(t_{k-1} - t) + (g'(\eta_{1k}) - g'(t))(t_{k-1} - t), \\
 g(t_k) &= g(t) + g'(t)(t_k - t) + (g'(\hat{\eta}_{1k}) - g'(t))(t_k - t),
 \end{aligned}$$

where $\eta_{1k}, \hat{\eta}_{1k} \in (t_{k-1}, t_k)$. Adding the above identities, we get

$$\begin{aligned}
 g(t) - \frac{g(t_{k-1}) + g(t_k)}{2} &= g'(t)(t - t_{k-\frac{1}{2}}) + \frac{1}{2}(g'(\eta_{1k}) - g'(t))(t - t_{k-1}) \\
 &\quad + \frac{1}{2}(g'(\hat{\eta}_{1k}) - g'(t))(t - t_k); \\
 g(t) - g(t_{n-1}) &= g'(\eta_{1n})(t - t_{n-1}), \quad \eta_{1n} \in (t_{n-1}, t_n).
 \end{aligned}$$

Then we have $R_n^{(1)} = R_{1n} + R_{2n} + R_{3n}$, where

$$R_{1n} = \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{g'(\tau)(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau, \quad R_{2n} = \frac{1}{\Gamma(\alpha)} \int_{t_{n-1}}^{t_n} \frac{g'(\eta_{1n})(\tau - t_{n-1})}{(t_n - \tau)^{1-\alpha}} d\tau,$$

$$R_{3n} = \frac{1}{2\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{(g'(\eta_{1k}) - g'(\tau))(\tau - t_{k-1})}{(t_n - \tau)^{1-\alpha}} + \frac{(g'(\hat{\eta}_{1k}) - g'(\tau))(\tau - t_k)}{(t_n - \tau)^{1-\alpha}} d\tau.$$

Now we estimate R_{1n} . We have

$$|R_{1n}| \leq \left| \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{(g'(\tau) - g'(t_{k-\frac{1}{2}}))(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau \right|$$

$$+ \left| \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{g'(t_{k-\frac{1}{2}})(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau \right|.$$

By the condition (5.3), we get

$$(5.7) \quad \left| \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{(g'(\tau) - g'(t_{k-\frac{1}{2}}))(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau \right|$$

$$\leq L \left| \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{(\tau - t_{k-\frac{1}{2}})^{1+\beta}}{(t_n - \tau)^{1-\alpha}} d\tau \right| \leq Ch^{1+\beta}.$$

Denote that $C_{n,k}^\alpha = \int_{t_{k-1}}^{t_k} \frac{(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau$. We have then

$$C_{n,k}^\alpha = \int_{t_{k-1}}^{t_{k-\frac{1}{2}}} \frac{(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau + \int_{t_{k-\frac{1}{2}}}^{t_k} \frac{(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau$$

$$= \frac{\int_{t_{k-1}}^{t_{k-1/2}} (t - t_{k-\frac{1}{2}}) dt}{(t_n - \bar{\xi}_k)^{1-\alpha}} + \frac{\int_{t_{k-1/2}}^{t_k} (t - t_{k-\frac{1}{2}}) dt}{(t_n - \tilde{\xi}_k)^{1-\alpha}},$$

where $t_{k-1} \leq \bar{\xi}_k \leq t_{k-1/2}$ and $t_{k-1/2} \leq \tilde{\xi}_k \leq t_k$. Thus we obtain

$$|C_{n,k}^\alpha| \leq \frac{h^2}{8} [(t_n - \tilde{\xi}_k)^{\alpha-1} - (t_n - \bar{\xi}_k)^{\alpha-1}].$$

It then follows that

$$(5.8) \quad \left| \sum_{k=1}^{n-1} g'(t_{k-\frac{1}{2}}) \left(\int_{t_{k-1}}^{t_k} \frac{(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau \right) \right|$$

$$\leq \frac{h^2}{8} \max_{t_0 \leq t \leq t_{n-1}} |g'(t)| \sum_{k=1}^{n-1} [(t_n - \tilde{\xi}_k)^{\alpha-1} - (t_n - \bar{\xi}_k)^{\alpha-1}] \leq Ch^{1+\alpha}.$$

Thus, by (5.7) and (5.8) we get $|R_{1n}| \leq Ch^{1+\min\{\alpha,\beta\}}$.

The estimate of R_{2n} is straightforward. Since $g \in C^1[0, T]$, we have

$$|R_{2n}| \leq \frac{1}{\Gamma(\alpha)} \int_{t_{n-1}}^{t_n} \frac{|g'(\eta_{1n})|(\tau - t_{n-1})}{(t_n - \tau)^{1-\alpha}} d\tau \leq Ch^{1+\alpha}.$$

Similarly to (5.7), we obtain that

$$R_{3n} \leq \left| \frac{L}{2\Gamma(\alpha)} \sum_{k=1}^{n-1} \left(\int_{t_{k-1}}^{t_k} \frac{(\tau - t_{k-1})^{1+\beta}}{(t_n - \tau)^{1-\alpha}} d\tau + \int_{t_{k-1}}^{t_k} \frac{(t_k - \tau)^{1+\beta}}{(t_n - \tau)^{1-\alpha}} d\tau \right) \right| \leq Ch^{1+\beta}.$$

Then we get the first estimate in (5.4). The estimate for $R_n^{(2)}$ can be proved similarly and we omit the proof here. \square

Proof of Lemma 5.2. By the Taylor expansion, we have for $t \in [t_{k-1}, t_k]$, $t \neq t_0$, that

$$t^p = \frac{t_k^p + t_{k-1}^p}{2} + pt_{k-\frac{1}{2}}^{p-1}(t - t_{k-\frac{1}{2}}) + \frac{p(p-1)}{2}(\eta_{2k})^{p-2}(t - t_{k-\frac{1}{2}})^2 - \frac{p(p-1)}{2}h^2[(\hat{\eta}_{2k})^{p-2} + (\bar{\eta}_{2k})^{p-2}], \eta_{2k}, \hat{\eta}_{2k}, \bar{\eta}_{2k} \in (t_{k-1}, t_k),$$

and $t^p = t_{n-1}^p + p(\eta_{2n})^{p-1}(t - t_{n-1})$, $t \in [t_{n-1}, t_n]$, $\eta_{2n} \in (t_{n-1}, t_n)$. Then we have $R_n^{(1)} = R_{1n} + R_{2n} + R_{3n} + R_{4n}$, and

$$\begin{aligned} R_{1n} &= \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{pt_{k-\frac{1}{2}}^{p-1}(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau, \\ R_{2n} &= \frac{p(p-1)}{2\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{(\eta_{2k})^{p-2}(\tau - t_{k-\frac{1}{2}})^2}{(t_n - \tau)^{1-\alpha}} d\tau, \\ R_{3n} &= -\frac{p(p-1)h^2}{2\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{[(\hat{\eta}_{2k})^{p-2} + (\bar{\eta}_{2k})^{p-2}]}{(t_n - \tau)^{1-\alpha}} d\tau, \\ R_{4n} &= \frac{1}{\Gamma(\alpha)} \int_{t_{n-1}}^{t_n} \frac{p(\eta_{2n})^{p-1}(\tau - t_{n-1})}{(t_n - \tau)^{1-\alpha}} d\tau. \end{aligned}$$

Similarly to the proof of (5.8), we have

$$\begin{aligned} |R_{1n}| &= \frac{1}{\Gamma(\alpha)} \left| \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{pt_{k-\frac{1}{2}}^{p-1}(\tau - t_{k-\frac{1}{2}})}{(t_n - \tau)^{1-\alpha}} d\tau \right| \leq \frac{p}{\Gamma(\alpha)} \sum_{k=1}^{n-1} t_{k-\frac{1}{2}}^{p-1} C_{n,k}^\alpha \\ &\leq \frac{ph^{\alpha+p}|\alpha-1|}{2\Gamma(\alpha)} \sum_{k=1}^{n-1} \left(k - \frac{1}{2}\right)^{p-1} (n-k)^{\alpha-2} \\ &\leq C_{\alpha,p}h^{\alpha+p}n^{\alpha+p-2} = C_{\alpha,p}h^2t_n^{\alpha+p-2}. \end{aligned}$$

By the mean value theorem and the Euler–Maclaurin formula, we obtain

$$\begin{aligned} |R_{2n}| &\leq \left| \frac{p(p-1)}{2\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \frac{(\eta_{2k})^{p-2}(\tau - t_{k-\frac{1}{2}})^2}{(t_n - \tau)^{1-\alpha}} d\tau \right| \\ &\leq \frac{|p(p-1)|}{2\Gamma(\alpha)} \sum_{k=1}^{n-1} (t_{k-1})^{p-2} \int_{t_{k-1}}^{t_k} \frac{(\tau - t_{k-\frac{1}{2}})^2}{(t_n - \tau)^{1-\alpha}} d\tau \\ &\leq \frac{|p(p-1)|h^p}{2\alpha\Gamma(\alpha)} \sum_{k=1}^{n-1} (k-1)^{p-2} [(t_n - t_{k-1})^\alpha - (t_n - t_k)^\alpha] \\ &\leq \frac{|p(p-1)|h^{p+\alpha}}{2\Gamma(\alpha)} \sum_{k=1}^{n-1} (k-1)^{p-2} (n-k-1)^{\alpha-1} \leq C_{\alpha,p}h^2t_n^{\alpha+p-2}. \end{aligned}$$

Similarly, we have $|R_{3n}| \leq C_{\alpha,p} h^2 t_n^{\alpha+p-2}$. Last, we estimate R_{4n} :

$$|R_{4n}| \leq \frac{ph}{\Gamma(\alpha)} (\eta_{2n})^{p-1} \int_{t_{n-1}}^{t_n} \frac{d\tau}{(t_n - \tau)^{1-\alpha}} \leq C_{\alpha,p} h^{1+\alpha} t_n^{p-1}.$$

By the estimates of $R_{1n}, R_{2n}, R_{3n}, R_{4n}$, we reach (5.5). The estimate (5.6) can be proved similarly. \square

5.2. Proof of Theorem 2.2. Denote the local truncation error $R_n^L = u(t_n) - u^*(t_n)$, $1 \leq n \leq N$, where

$$\begin{aligned} (5.9) \quad u^*(t_n) &= u_0 + A \sum_{k=1}^{n-1} \frac{u(t_{k-1}) + u(t_k)}{2} ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k) + Au(t_n)(I_{t_{n-1}}^\alpha 1)(t_n) \\ &\quad + \sum_{k=1}^{n-1} f\left(t_{k-\frac{1}{2}}, \frac{u(t_{k-1}) + u(t_k)}{2}\right) ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k) \\ &\quad + f(t_{n-1}, u(t_{n-1}))(I_{t_{n-1}}^\alpha 1)(t_n). \end{aligned}$$

LEMMA 5.3 (local error of the scheme TS-I). *Suppose that $u \in C^2([0, T])$ and $f(t, u)$ in (2.1) satisfies the Lipschitz condition (2.2). Then there exists a constant C independent of the step size h such that the local truncation error of the TS-I scheme (2.18)–(2.21) satisfies*

$$(5.10) \quad |R_n^L| = |u(t_n) - u^*(t_n)| \leq C(1 + |u'(0)|t_n^{-\alpha})h^{1+\alpha}.$$

Otherwise, if we assume $f \in C^2(G)$, then there exists a constant C independent of the step size h such that the local truncation error of the TS-I scheme (2.18)–(2.21) satisfies

$$(5.11) \quad |R_n^L| = |u(t_n) - u^*(t_n)| \leq C(1 + t_n^{\alpha-1})h^{1+\alpha}.$$

Proof. Subtracting (5.9) from (2.4) we get $R_n^L = R_n^u + R_n^f$, where

$$\begin{aligned} |R_n^u| &= \left| (I_{t_0}^\alpha Au)(t_n) - \sum_{k=1}^{n-1} \frac{A(u(t_{k-1}) + u(t_k))}{2} ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k) - Au(t_n)(I_{t_{n-1}}^\alpha 1)(t_n) \right|, \\ |R_n^f| &= \left| (I_{t_0}^\alpha f)(t, u(t)) - \sum_{k=1}^{n-1} f\left(t_{k-\frac{1}{2}}, \frac{u(t_{k-1}) + u(t_k)}{2}\right) ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k) \right. \\ &\quad \left. - f(t_{n-1}, u(t_{n-1}))(I_{t_{n-1}}^\alpha 1)(t_n) \right|. \end{aligned}$$

We first prove the estimate (5.10). Due to the assumption $u \in C^2[0, T]$, by Lemma 5.1, we have $|R_n^u| \leq Ch^{1+\alpha}$. Furthermore, it can be readily checked by Taylor's expansion (see also [9, Theorem 2.2]) that for all $t_1, t_2 \in [0, T]$,

$$(5.12) \quad \begin{aligned} |f(t_1, u(t_1)) - f(t_2, u(t_2))| &= |[{}^C D_0^\alpha u](t_1) - [{}^C D_0^\alpha u](t_2) + Au(t_2) - Au(t_1)| \\ &\leq K_1 |u'(0)| |t_1 - t_2|^\beta + K_1 |t_1 - t_2|, \end{aligned}$$

where $\beta = 1 - \alpha$ and K_1 is a positive constant. Using the Hölder continuous condition (5.12) and the Lipschitz continuous condition (2.2), we have

$$\begin{aligned}
 |R_n^f| \leq & \frac{1}{\Gamma(\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \left(K_1 |u'(0)| |\tau - t_{k-\frac{1}{2}}|^{1-\alpha} + K_1 |\tau - t_{k-\frac{1}{2}}| \right. \\
 & \left. + K \left| u(\tau) - \frac{u(t_{k-1}) + u(t_k)}{2} \right| \right) (t_n - \tau)^{\alpha-1} d\tau \\
 & + \frac{1}{\Gamma(\alpha)} \int_{t_{n-1}}^{t_n} \left(K_1 |u'(0)| |\tau - t_{n-1}|^{1-\alpha} \right. \\
 (5.13) \quad & \left. + K_1 |\tau - t_{n-1}| + K |u(\tau) - u(t_{n-1})| \right) (t_n - \tau)^{\alpha-1} d\tau.
 \end{aligned}$$

By (5.13) and Lemmas 5.1 and 5.2, we have

$$|R_n^f| \leq C_1 h^{1+\alpha} + C_2 |u'(0)| \max\{h^2 t_n^{-1}, h^{1+\alpha} t_n^{-\alpha}\} \leq C(1 + |u'(0)| t_n^{-\alpha}) h^{1+\alpha}.$$

Now we prove the estimate (5.11). By Lemmas 5.1 and 5.2, it is readily checked from (2.25) that

$$|R_n^u| \leq C_3 \max\{h^2 t_n^{2\alpha-2}, h^{1+\alpha} t_n^{\alpha-1}\} \leq C t_n^{\alpha-1} h^{1+\alpha}.$$

Due to the smoothness of f , (5.12) holds with $\beta = 1$ in this case. Following the proof of Lemma 5.1 and by Lemma 5.2, we have $|R_n^f| \leq C(1 + t_n^{\alpha-1}) h^{1+\alpha}$. \square

Now, we are in the position to prove Theorem 2.2. Denote $e_n = u(t_n) - \tilde{u}_n$. Recall that

$$(5.14) \quad I - A(I_{t_{n-1}}^\alpha 1)(t_n) = I - \frac{Ah^\alpha}{\Gamma(1 + \alpha)} = C_h^\alpha.$$

Feeding (2.19) into (2.18), and substituting the resulting identity and (2.21) into (2.20), we get

$$\begin{aligned}
 \tilde{u}_n = & u_0 + A \sum_{k=1}^{n-1} \frac{\tilde{u}_{k-1} + \tilde{u}_k}{2} ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k) + A\tilde{u}_n (I_{t_{n-1}}^\alpha 1)(t_n) \\
 (5.15) \quad & + \sum_{k=1}^{n-1} f\left(t_{k-\frac{1}{2}}, \frac{\tilde{u}_{k-1} + \tilde{u}_k}{2}\right) ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k) + f(t_{n-1}, \tilde{u}_{n-1})(I_{t_{n-1}}^\alpha 1)(t_n).
 \end{aligned}$$

By (5.15), (5.9), and (5.14), we have

$$\begin{aligned}
 C_h^\alpha e_n = & R_n^L + A \sum_{k=1}^{n-1} \frac{e_{k-1} + e_k}{2} ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k) \\
 & + \left(f(t_{n-1}, u(t_{n-1})) - f(t_{n-1}, \tilde{u}_{n-1}) \right) (I_{t_{n-1}}^\alpha 1)(t_n) \\
 & + \sum_{k=1}^{n-1} \left(f\left(t_{k-\frac{1}{2}}, \frac{u(t_{k-1}) + u(t_k)}{2}\right) - f\left(t_{k-\frac{1}{2}}, \frac{\tilde{u}_{k-1} + \tilde{u}_k}{2}\right) \right) ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k).
 \end{aligned}$$

Using the Lipschitz condition (2.2), it follows that

$$\begin{aligned} |C_h^\alpha e_n| &\leq |R_n^L| + (\|A\| + K) \sum_{k=1}^{n-1} \frac{|e_{k-1}| + |e_k|}{2} ({}_{[t_n]}I_{t_{k-1}}^\alpha 1)(t_k) + K|e_{n-1}|({}_n I_{t_{n-1}}^\alpha 1)(t_n) \\ &\leq |R_n^L| + \frac{(\|A\| + 2K)h^\alpha}{\Gamma(1 + \alpha)} \left[(n^\alpha - (n - 1)^\alpha)|e_0| + \sum_{k=1}^{n-1} ((n - k + 1)^\alpha - (n - k - 1)^\alpha)|e_k| \right]. \end{aligned}$$

By the mean value theorem, we obtain that

$$\|C_h^\alpha\| |e_n| \leq |R_n^L| + \frac{2\alpha(\|A\| + 2K)h^\alpha}{\Gamma(1 + \alpha)} \sum_{k=0}^{n-1} \frac{|e_k|}{(n - k)^{1-\alpha}}.$$

Then by Lemma 5.3 and the singular Gronwall inequality [12], for $u \in \mathcal{C}^2[0, T]$, we have for $1 \leq n \leq N$

$$(5.16) \quad |e_n| \leq C(1 + |u'(0)|t_n^{-\alpha})h^{1+\alpha}E_\alpha[M\Gamma(\alpha)T^\alpha],$$

and for $f \in \mathcal{C}^2(G)$, we have for $1 \leq n \leq N$

$$(5.17) \quad |e_n| \leq C(1 + t_n^{\alpha-1})h^{1+\alpha}E_\alpha[M\Gamma(\alpha)T^\alpha],$$

where $E_\alpha[z] = \sum_{k=0}^\infty \frac{z^k}{\Gamma(k\alpha+1)}$ is the well-known Mittag-Leffler function, and $M = \frac{2\alpha}{c_0}(\|A\| + 2K)$. This completes the proof of Theorem 2.2. \square

Remark 5.4. In the proof, we merge the scheme (2.18)–(2.21) and obtain (5.15) and compare with the integral equation (2.4), where neither $\bar{u}(t_n)$ nor \bar{u}_n are present. In other words, \bar{u}_n is merely an intermediate step in the computation. Recall from Remarks 2.1 and 2.5 that \bar{u} is not a numerical solution.

Remark 5.5 (uniform convergence). For a solution $u \in \mathcal{C}^2[0, T]$, if $f(t, u)$ satisfies the Lipschitz condition with respect to all arguments, or $u'(0) = 0$, then in (5.12), the order of the Hölder continuous condition will be $\beta = 1$. Then we can obtain by Lemma 5.1 that $\max_{1 \leq n \leq N} |R_n^L| \leq Ch^{1+\alpha}$. Consequently, we will have uniform convergence of order $1 + \alpha$:

$$\max_{1 \leq n \leq N} |e_n| \leq Ch^{1+\alpha}E_\alpha[M\Gamma(\alpha)T^\alpha].$$

6. Conclusion. We have presented two time-splitting methods (three time-splitting schemes) for time-fractional differential equations with smooth solution: the first two schemes are based on an integral form of the time-fractional differential equations and are of order $1 + \alpha$ (TS-I) and α (TS-II), respectively, while the third one is of order $2 - \alpha$ (TS-III). We numerically show that the two schemes of order $1 + \alpha$ and $2 - \alpha$ for a linear test equation are $A(\frac{\alpha\pi}{2})$ -stable.

We observe that for some nonsmooth solutions, the TS-I scheme is still of order $1 + \alpha$ while the TS-III scheme is only of order $1 - \alpha$. We also tested the TS-I and TS-III schemes for a time-fractional reaction-diffusion equation with the Fourier spectral method in physical space: the TS-I scheme is of order $1 + \alpha$ while the TS-III scheme is of order one at the final time. This is consistent with our observation in Remark 2.9

where a simple linear equation is considered: the TS-I scheme requires less smoothness than the TS-III scheme does.

Moreover, we use a substepping TS-I scheme for solving a stiff system and the numerical results show that for the same level of accuracy, the substepping TS-I scheme costs less than half the computational time of that of the TS-I scheme without substepping.

In this work, we mainly focus on smooth solutions (with bounded first two derivatives) while the solutions to fractional differential equations may not have that regularity. These schemes are not uniformly convergent unless we have strict requirements on regularity of solutions or forcing terms. The errors at the starting point can be large and thus may pollute the accuracy away from the starting point. In subsequent work, we will focus on nonsmooth solutions and propose higher-order numerical methods of uniform convergence.

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