

# Implicit-Explicit difference schemes for nonlinear fractional differential equations with non-smooth solutions

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## Abstract

We propose second-order implicit-explicit (IMEX) time-stepping schemes for nonlinear fractional differential equations with fractional order  $0 < \beta < 1$ . From the known structure of the non-smooth solution and by introducing corresponding correction terms, we can obtain uniformly second-order accuracy from these schemes. We prove the convergence and linear stability of the proposed schemes. Numerical examples illustrate the flexibility and efficiency of the IMEX schemes and show that they are effective for nonlinear and multi-rate fractional differential systems as well as multi-term fractional differential systems with non-smooth solutions.

**Keywords** time-fractional derivatives, IMEX schemes, low regularity, multi-rate systems, multi-term fractional derivatives

## 1 Introduction

We aim at constructing efficient finite difference schemes for fractional ordinary differential equations (FODEs) with non-smooth solutions. In recent decades, due to the increasing interest in problems with anomalous transport dynamics, fractional differential equations have become significant mathematical models in many fields of science and engineering, such as viscoelastic models in blood flow [33], underground transport [20], options pricing model in financial markets [41], etc.

Though some fractional differential equations (FDEs) with special form, e.g., linear equations, can be solved by analytical methods, e.g., the Fourier transform method or the Laplace transform method [34], the analytical solutions of many generalized FDEs (e.g. nonlinear FDEs and multi-term FDEs) are rather difficult to obtain. This encourages us to develop effective numerical methods for solutions of these FDEs. Up to now, a number of finite difference methods have been established for FDEs. One way is to transform the considered FDEs into their integral forms, then numerical methods for the fractional integral operator are developed and the corresponding difference schemes are derived; see [4, 5, 10, 11, 17, 18, 15, 29, 30, 37, 48]. Another approach is to approximate the fractional derivative operators in the considered FDEs directly; see [16, 27, 36, 38, 54]. Besides finite difference methods, there exist also other numerical methods for FDEs, e.g., finite element methods [22, 40], spectral methods [26, 39, 45], matrix methods [32, 35], etc.

For nonlinear FDEs, most of the aforementioned finite difference methods are implicit, and the nonlinear system needs to be solved using the iteration method, which is costly. To avoid extra computational costs

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and instability caused by iteration, various numerical methods have been proposed, e.g., predictor-corrector methods; see [6, 7, 10, 11, 17, 25, 42, 53] and time-splitting schemes [1].

Implicit-explicit (IMEX) schemes (also known as semi-implicit schemes, linearly-implicit schemes) play a major role in the numerical treatment of nonlinear/stiff differential equations [12, 21, 24]. Due to approximating the nonlinear/nonstiff part explicitly, we avoid solving nonlinear equations/systems in every time step, and hence the computational cost can be reduced significantly. Moreover, the IMEX schemes generally have better stability than explicit schemes, for the linear/stiff parts are treated implicitly. To the best of authors' knowledge, there are very limited works on IMEX schemes for FDEs. An IMEX scheme has been proposed for nonlinear fractional anomalous diffusion equations with smooth solutions in [47] and an explicit and implicit finite difference scheme for fractional Cattaneo equation was developed in [19]. Some semi-implicit methods for space-fractional differential equations can be found in the literature, e.g., see [3, 28, 43].

The main contribution of this work is to develop second-order IMEX schemes for nonlinear/stiff FODEs with solutions that have a weak singularity at the origin. Most numerical methods for differential equations are generally intended for problems with solutions of high regularity. However, solutions to FDEs usually have weak singularities at the origin even when the forcing term is smooth, see e.g. [9, 11, 23]. When solving these FDEs, the singularity requires special attention to obtain the expected high accuracy. Several approaches have been proposed to deal with the weak singularity, such as using adaptive grids (nonuniform grids) to keep errors small near the singularity [18, 44, 51], or employing non-polynomial basis functions to include the correct singularity index [2, 14, 52], or using the correction terms to remedy the loss of accuracy and recover high-order schemes [18, 30, 46, 49, 50].

In this paper, we follow the last approach to develop IMEX methods with uniformly second-order accuracy for FODEs, whose solutions are non-smooth and have known structure. To deal with the singularity, we apply correction terms in the proposed schemes, so that the resulting fractional quadratures are either exact or sufficiently accurate for the weakly singular parts of the solutions. The idea of adding correction terms was firstly proposed for approximating fractional-order integrals by the linear multi-step method in [30]. Very recently, the same strategy has been adopted to enhance the accuracy of numerical schemes for FDEs [49, 50]. To treat the nonlinear part explicitly, we further use extrapolation and Taylor expansion to approximate the nonlinear part, where appropriate correction terms are also used to obtain high accuracy for non-smooth solutions. We propose two IMEX schemes, which can work for nonlinear/stiff FODEs with uniformly second-order convergence, even when the solutions have weak singularity at the origin. We also prove the convergence and linear stability of the proposed schemes.

We organize this work as follows. In Section 2, we formulate the IMEX method based on the fractional linear multistep method (FLMM), and then derive two IMEX schemes by applying the extrapolation and Taylor expansion for the nonlinear terms. Moreover, we provide the strategies for introducing correction terms to the schemes to make them uniformly second-order for FODEs with non-smooth solutions. We also present convergence rates of the proposed schemes, the proofs of which are given in Section 6. In Section 3, we discuss the linear stability of the proposed schemes. We present more details on the proposed IMEX schemes in Section 4 to show that they can be applied to stiff systems and multi-term nonlinear FODEs. In Section 5, we present numerical examples to illustrate the computational flexibility and verify our error estimates. We conclude in Section 7 and discuss the performance of the proposed schemes.

## 2 Second-order IMEX schemes

We consider the following nonlinear FODE

$$({}^C D_0^\beta u)(t) = \lambda u(t) + f_u(t), \quad t \in (0, T], \quad u(0) = u_0, \quad (2.1)$$

where  $0 < \beta < 1$ ,  $f_u(t) = f(t, u(t))$ ,  ${}^C D_0^\beta$  is the Caputo derivative defined by

$$({}^C D_a^\beta g)(t) = (I_a^{1-\beta} g')(t), \quad (I_a^\beta g)(t) = \frac{1}{\Gamma(\beta)} \int_a^t \frac{g(\tau)}{(t-\tau)^{1-\beta}} d\tau, \quad t > a. \quad (2.2)$$

We first transform (2.1) into its integral form as

$$u(t) = u(0) + \lambda (I_0^\beta u)(t) + (I_0^\beta f_u)(t), \quad 0 \leq t \leq T. \quad (2.3)$$

Eq. (2.3) is readily obtained by applying the operator  $I_0^\beta$  on both sides of (2.1) and using the identity  $(I_a^\beta {}^C D_a^\beta g)(t) = g(t) - g(a)$ , see, e.g. [11].

In order to obtain second-order schemes, we need to approximate the fractional integrals in (2.3) with second-order quadrature rules. However, the solutions to (2.1) usually have singularity at  $t = 0$ . The analytical solution to (2.1) can be written as the summation of regular and singular parts, as given in the following lemma. See also [8, 9, 11] for more discussions.

**Lemma 2.1** ([11]) *Suppose  $f \in \mathcal{C}^3(G)$ , where  $G$  is a suitable region of variable  $u$ . Then there exists a function  $\psi \in \mathcal{C}^2[0, T]$  and some  $c_1, \dots, c_{\hat{\nu}} \in \mathbb{R}$  and  $d_1, \dots, d_{\hat{\eta}} \in \mathbb{R}$ , such that the solution of (2.1) is of the form*

$$u(t) = \psi(t) + \sum_{\nu=1}^{\hat{\nu}} c_\nu t^{\nu\beta} + \sum_{\eta=1}^{\hat{\eta}} d_\eta t^{1+\eta\beta}, \quad (2.4)$$

where  $\hat{\nu} := [2/\beta] - 1$ ,  $\hat{\eta} := [1/\beta] - 1$ .

The solution of (2.1) is usually non-smooth, even if  $f(t, u(t))$  is smooth. Consequently, many existing numerical methods (see e.g. [10, 18, 47]) for (2.1) would produce less accurate numerical solutions when they are directly applied. Next, we will adopt a second-order FLMM developed in [30] to (2.3) to construct our IMEX schemes. Take a uniform partition of time interval  $[0, T]$ , i.e.,  $t_n = nh, 0 \leq n \leq N$  with  $h = T/N$ . The second-order FLMM used in the present work reads

$$I_0^\beta u(t_n) = h^\beta \sum_{j=0}^n \omega_{n-j}^{(\beta)} u(t_j) + h^\beta \sum_{j=0}^m W_{n,j}^{(\beta)} u(t_j) + O(h^2), \quad (2.5)$$

where  $\{\omega_j^{(\beta)}\}$  are coefficients of the Taylor expansion of the following generating function

$$\omega^{(\beta)}(z) = \left( \frac{1}{2} \frac{1+z}{1-z} \right)^\beta = \sum_{j=0}^{\infty} \omega_j^{(\beta)} z^j, \quad (2.6)$$

and  $\{W_{n,j}^{(\beta)}\}$  are the starting weights that recover second-order accuracy. If we drop the correction terms  $\sum_{j=0}^m W_{n,j}^{(\beta)} u(t_j)$  in (2.5), then we would lose the second-order accuracy, unless  $u(t)$  satisfies some special conditions, i.e.,  $u(t)$  is smooth and  $u(0) = u'(0) = 0$ .

The following lemma states the convergence of (2.5) with no correction terms.

**Lemma 2.2** ([30, 48]) *If  $u(t) = t^\nu$ ,  $\nu \geq 0$ , then for (2.5) with  $m = 0$ ,*

$$(I_0^\beta u)(t_n) = h^\beta \sum_{k=0}^n \omega_{n-k}^{(\beta)} u(t_k) + O(h^2 t_n^{\nu+\beta-2}) + O(h^{1+\nu} t_n^{\beta-1}), \quad (2.7)$$

where  $\{\omega_k^{(\beta)}\}$  are defined by (2.6).

From Lemma 2.1, we see that the analytical solution of FODE (2.1) has the form of (2.4) when  $f(t, u(t))$  satisfies some suitable conditions. In the following, we will always assume that  $u(t)$  can be expressed in the following form for convenience,

$$u(t) - u(0) = \sum_{r=1}^{m+1} c_r t^{\sigma_r} + \xi(t) t^{\sigma_{m+2}}, \quad 0 < \sigma_r < \sigma_{r+1}, \quad (2.8)$$

where  $\xi(t)$  is a uniformly continuous function over the interval  $[0, T]$  and  $c_r \in \mathbb{R}$  are constants. The sequence  $\{\sigma_r\}$  is uniquely determined by the considered equation. For example, when  $f_u(t) = f(t)$  in (2.1) is smooth,  $\sigma_r$ 's are of the form  $\{i + j\beta\}$ , see [34, Chapter 5]. Another example is from Lemma 2.1,  $\sigma_r$ 's are of the form (2.4).

Given a sequence of positive numbers  $\{\theta_r\}$ , we define the operator  $I_{h,\theta}^{\beta,n,m}$  as

$$I_{h,\theta}^{\beta,n,m} g = h^\beta \sum_{k=0}^n \omega_{n-k}^{(\beta)} g(t_k) + h^\beta \sum_{k=1}^m W_{n,k}^{(\beta,\theta)} g(t_k) + h^\beta B_n^\theta g(t_0), \quad (2.9)$$

where  $\omega_k^{(\beta)}$  satisfies (2.6), and  $W_{n,k}^{(\beta,\theta)}$  and  $B_n^\theta$  are given by

$$\sum_{k=1}^m W_{n,k}^{(\beta,\theta)} k^{\theta_r} = \frac{\Gamma(\theta_r + 1)}{\Gamma(\theta_r + 1 + \beta)} n^{\theta_r + \beta} - \sum_{k=0}^n \omega_{n-k}^{(\beta)} k^{\theta_r}, \quad 1 \leq r \leq m, \quad (2.10)$$

$$B_n^\theta = \frac{n^\beta}{\Gamma(1 + \beta)} - \sum_{k=0}^n \omega_{n-k}^{(\beta)} - \sum_{k=1}^m W_{n,k}^{(\beta,\theta)}. \quad (2.11)$$

Here  $W_{n,k}^{(\beta,\theta)}$  in (2.9) are called the starting weights that are chosen such that  $I_{h,\theta}^{\beta,n,m} g = (I_0^\beta g)(t_n)$  when  $g(t) = t^{\theta_r}$  ( $1 \leq r \leq m$ ), which leads to (2.10).

**Remark 2.3** The linear system (2.10) is ill-conditioned when  $m$  is large [8, 30, 50]. The large condition number of the Vandermonde-type matrix in (2.10) may lead to big roundoff errors of the starting weights  $W_{n,k}^{(\beta,\theta)}$  ( $1 \leq k \leq m$ ). However, we do not need many correction terms to get satisfactory numerical solutions in computation as observed in [50]. With this observation, we only need to solve the system (2.10) with moderately large condition number. Thus we can obtain reasonable accuracy of the starting weights and hence the numerical solutions, see [8, 50]. We present residuals of the system (2.10) and its corresponding condition numbers in Example 5.1 and Example 5.2.

If we apply (2.9) to approximate  $I_0^\beta u(t)$ , where  $u(t)$  satisfies (2.8), then by (2.7) we have

$$\begin{aligned} (I_0^\beta u)(t_n) &= (I_0^\beta (u - u(0)))(t_n) + \frac{t_n^\beta u(0)}{\Gamma(1 + \beta)} \\ &= h^\beta \sum_{k=0}^n \omega_{n-k}^{(\beta)} (u(t_k) - u_0) + h^\beta \sum_{k=1}^{m_u} W_{n,k}^{(\beta,\sigma)} (u(t_k) - u_0) + \frac{t_n^\beta u_0}{\Gamma(1 + \beta)} + R_u^n \\ &= I_{h,\sigma}^{\beta,n,m_u} u + R_u^n, \end{aligned} \quad (2.12)$$

where  $I_{h,\sigma}^{\beta,n,m_u}$  is defined by (2.9) and  $R_u^n$  is defined by

$$R_u^n = O(h^2 t_n^{\sigma_{m_u+1} + \beta - 2}) + O(h^{1 + \sigma_{m_u+1}} t_n^{\beta - 1}). \quad (2.13)$$

From (2.1), we have

$$f_u(t) = f(t, u(t)) = ({}^C D_0^\beta u)(t) - \lambda u(t). \quad (2.14)$$

Hence, the regularity of  $f(t, u(t))$  is related to the regularity of  $u$ . In fact, based on the smoothness assumption of  $u(t)$  (see Eq. (2.8)), we obtain that  $f(t, u(t))$  has the form

$$\begin{aligned} f(t, u(t)) - f(0, u(0)) &= -\lambda \sum_{r=1}^{m+1} c_r t^{\sigma_r} + \sum_{r=1}^{m+1} c_r \frac{\Gamma(\sigma_r + 1)}{\Gamma(\sigma_r + 1 - \beta)} t^{\sigma_r - \beta} + \dots \\ &= \sum_{r=1}^{l+1} d_r t^{\delta_r} + \zeta(t) t^{\delta_{l+2}}, \end{aligned} \quad (2.15)$$

where  $\zeta(t)$  is uniformly bounded on  $[0, T]$ ,  $\delta_r < \delta_{r+1}$ , and  $\delta_r \in \{\sigma_k, k \geq 1\} \cup \{\sigma_k - \beta, k \geq 1\}$  with  $\sigma_k$ 's from (2.8).

Similar to (2.12), we have

$$(I_{t_0}^\beta f_u)(t_n) = I_{h,\delta}^{\beta,n,m_f} f_u + R_f^n, \quad (2.16)$$

where  $I_{h,\delta}^{\beta,n,m_f}$  is defined by (2.9),

and the truncation error  $R_f^n$  is given by

$$R_f^n = O(h^2 t_n^{\delta_{m_f+1} + \beta - 2}) + O(h^{1 + \delta_{m_f+1}} t_n^{\beta - 1}). \quad (2.17)$$

From (2.12) and (2.16), we can derive the following implicit discretization for (2.3)

$$u(t_n) = u_0 + \lambda I_{h,\sigma}^{\beta,n,m_u} u + I_{h,\delta}^{\beta,n,m_f} f_u + R_u^n + R_f^n, \quad (2.18)$$

where  $I_{h,\sigma}^{\beta,n,m_u}$  and  $I_{h,\delta}^{\beta,n,m_f}$  are defined by (2.9),  $R_u^n$  and  $R_f^n$  are defined by (2.13) and (2.17), respectively.

Let  $U_k$  be the approximate solution of  $u(t_k)$ . Dropping the truncation errors  $R_u^n$  and  $R_f^n$  in (2.18) and replacing  $u(t_k)$  with  $U_k$ , we derive the fully implicit method for (2.3): to find  $U_n$  for  $n = n_0, n_0 + 1, \dots$  such that

$$U_n = u_0 + \lambda I_{h,\sigma}^{\beta,n,m_u} U + I_{h,\delta}^{\beta,n,m_f} F, \quad (2.19)$$

where  $n_0 = 1 + \max\{m_f, m_u\}$ ,  $F_n = f(t_n, U_n)$ .

Given  $U_k$  ( $k = 0, 1, \dots, n-1$ ), we need to solve a nonlinear system (2.19) at each time step to get  $U_n$ . Next, we further use the extrapolation and Taylor expansion with correction terms to approximate  $f(t_n, u(t_n))$  in (2.18), which leads to linear systems and also preserves high-order accuracy.

If  $u(t) = t^\sigma$ ,  $\sigma > 0$ , then we have from the Taylor expansion that

$$u(t_n) = 2u(t_{n-1}) - u(t_{n-2}) + O(h^2 t_n^{\sigma-2}), \quad n \geq 2, \quad (2.20)$$

$$u(t_n) = u(t_{n-1}) + h u'(t_{n-1}) + O(h^2 t_n^{\sigma-2}), \quad n \geq 2. \quad (2.21)$$

(1) **By extrapolation with correction terms:** It is clear that (2.20) does not preserve globally second-order accuracy when  $\sigma < 2$ . Hence,  $2f(t_{n-1}, u(t_{n-1})) - f(t_{n-2}, u(t_{n-2}))$  is not a second-order approximation of  $f(t_n, u(t_n))$  when  $f(t, u(t))$  is not sufficiently smooth, see (2.15). By adding correction terms to (2.20), we can obtain

$$\begin{aligned} f(t_n, u(t_n)) &= 2f(t_{n-1}, u(t_{n-1})) - f(t_{n-2}, u(t_{n-2})) \\ &\quad + \sum_{k=1}^{\tilde{m}_f} \widehat{W}_{n,k}^{(f)} (f(t_k, u(t_k)) - f(t_0, u_0)) + \tilde{R}_f^n, \quad n \geq 2, \end{aligned} \quad (2.22)$$

where  $\{\widehat{W}_{n,k}^{(f)}\}$  are chosen such that the above equation (2.22) is exact, i.e.,  $\widetilde{R}_f^n = 0$ , for  $f(t, u(t)) = t^{\delta_r} (1 \leq r \leq \widetilde{m}_f)$ , i.e.,  $\{\widehat{W}_{n,k}^{(f)}\}$  satisfy

$$\sum_{k=1}^{\widetilde{m}_f} \widehat{W}_{n,k}^{(f)} k^{\delta_r} = n^{\delta_r} - 2(n-1)^{\delta_r} + (n-2)^{\delta_r}, \quad r = 1, \dots, \widetilde{m}_f. \quad (2.23)$$

The truncation error  $\widetilde{R}_f^n$  in (2.22) satisfies

$$\widetilde{R}_f^n = O(h^2 t_n^{\delta_{\widetilde{m}_f+1}-2}) \quad (2.24)$$

when  $f(t, u(t))$  satisfies (2.15).

Inserting (2.22) into (2.18) yields

$$\begin{aligned} u(t_n) = & u_0 + \lambda I_{h,\sigma}^{\beta,n,m_u} u + I_{h,\delta}^{\beta,n,m_f} f_u \\ & + h^\beta \omega_0^{(\beta)} \left[ -f(t_n, u(t_n)) + 2f(t_{n-1}, u(t_{n-1})) - f(t_{n-2}, u(t_{n-2})) \right. \\ & \left. + \sum_{k=1}^{\widetilde{m}_f} \widehat{W}_{n,k}^{(f)} (f(t_k, u(t_k)) - f(t_0, u_0)) \right] + R_E^n, \end{aligned} \quad (2.25)$$

where  $R_E^n = R_u^n + R_f^n + h^\beta \widetilde{R}_f^n$ ,  $R_u^n$ ,  $R_f^n$ , and  $\widetilde{R}_f^n$  are defined by (2.13), (2.17), and (2.24), respectively.

From (2.25), we obtain the IMEX method based on the extrapolation technique (abbreviated as **IMEX-E**) as: given  $U_k (0 \leq k \leq n-1)$ , to find  $U_n (n \geq 2)$  such that

$$\begin{aligned} U_n = & U_0 + \lambda I_{h,\sigma}^{\beta,n,m_u} U + I_{h,\delta}^{\beta,n,m_f} F - h^\beta \omega_0^{(\beta)} F_n \\ & + h^\beta \omega_0^{(\beta)} \left[ 2F_{n-1} - F_{n-2} + \sum_{k=1}^{\widetilde{m}_f} \widehat{W}_{n,k}^{(f)} (F_k - F_0) \right], \end{aligned} \quad (2.26)$$

where  $F_k = f(t_k, U_k)$ ,  $\omega_0^{(\beta)} = 2^{-\beta}$ ,  $I_{h,\sigma}^{\beta,n,m_u}$  and  $I_{h,\delta}^{\beta,n,m_f}$  are defined by (2.9), and  $\widehat{W}_{n,k}^{(f)}$  is given by (2.23).

**Remark 2.4** Given  $U_k (0 \leq k \leq n-1)$ , Eq. (2.26) is a linear equation of  $U_n$ . In fact,  $I_{h,\delta}^{\beta,n,m_f} F$  contains  $h^\beta \omega_0^{(\beta)} F_n$ , and it can be eliminated by the following term  $-h^\beta \omega_0^{(\beta)} F_n$  in the scheme.

(2) **By Taylor expansion with correction terms:** From the Taylor expansion and (2.21), we have

$$\begin{aligned} f(t_n, u(t_n)) = & f(t_{n-1}, u(t_{n-1})) + h f'(t_{n-1}, u(t_{n-1})) \\ & + \sum_{k=1}^{\widetilde{m}_f} \widehat{W}_{n,k}^{(f)} (f(t_k, u(t_k)) - f(t_0, u_0)) + O(h^2 t_n^{\delta_{\widetilde{m}_f+1}-2}), \quad n \geq 2, \end{aligned} \quad (2.27)$$

where  $f'(t_{n-1}, u(t_{n-1})) = \frac{d}{dt} f(t, u(t))|_{t=t_{n-1}}$ , and the starting weights  $\{\widehat{W}_{n,k}^{(f)}\}$  are chosen such that Eq. (2.27) is exact for  $f(t, u(t)) = t^{\delta_r} (1 \leq r \leq \widetilde{m}_f)$ , i.e.,  $\{\widehat{W}_{n,k}^{(f)}\}$  satisfy

$$\sum_{k=1}^{\widetilde{m}_f} \widehat{W}_{n,k}^{(f)} k^{\delta_r} = n^{\delta_r} - (n-1)^{\delta_r} - \delta_r (n-1)^{\delta_r-1}, \quad 1 \leq r \leq \widetilde{m}_f. \quad (2.28)$$

Next, we approximate  $f'(t_{n-1}, u(t_{n-1}))$  with correction terms, which is given by

$$\begin{aligned}
f'(t_{n-1}, u(t_{n-1})) &= \partial_u f(t_{n-1}, u(t_{n-1})) \partial_t u(t_{n-1}) + \partial_t f(t_{n-1}, u(t_{n-1})) \\
&= \partial_u f(t_{n-1}, u(t_{n-1})) \left[ \frac{u(t_n) - u(t_{n-1})}{h} + \frac{1}{h} \sum_{k=1}^{\tilde{m}_u} \widetilde{W}_{n,k}^{(u)} (u(t_k) - u_0) \right. \\
&\quad \left. + O(h t_n^{\sigma_{\tilde{m}_u+1}-2}) \right] + \partial_t f(t_{n-1}, u(t_{n-1})), \quad n \geq 2,
\end{aligned} \tag{2.29}$$

where  $\{\widetilde{W}_{n,k}^{(u)}\}$  are chosen such that

$$\frac{u(t_n) - u(t_{n-1})}{h} + \frac{1}{h} \sum_{k=1}^{\tilde{m}_u} \widetilde{W}_{n,k}^{(u)} (u(t_k) - u_0) = u'(t_{n-1})$$

for some  $u(t) = t^{\sigma_r}$  ( $1 \leq r \leq \tilde{m}_u$ ), i.e.,  $\{\widetilde{W}_{n,k}^{(u)}\}$  satisfy

$$\sum_{k=1}^{\tilde{m}_u} \widetilde{W}_{n,k}^{(u)} k^{\sigma_r} = \sigma_r (n-1)^{\sigma_r-1} - (n^{\sigma_r} - (n-1)^{\sigma_r}), \quad 1 \leq r \leq \tilde{m}_u. \tag{2.30}$$

Combining (2.27) and (2.29) yields

$$\begin{aligned}
f(t_n, u(t_n)) &= f(t_{n-1}, u(t_{n-1})) + h \partial_t f(t_{n-1}, u(t_{n-1})) \\
&\quad + \partial_u f(t_{n-1}, u(t_{n-1})) \left[ u(t_n) - u(t_{n-1}) + \sum_{k=1}^{\tilde{m}_u} \widetilde{W}_{n,k}^{(u)} (u(t_k) - u_0) \right] \\
&\quad + \sum_{k=1}^{\tilde{m}_f} \widetilde{W}_{n,k}^{(f)} (f(t_k, u(t_k)) - f(t_0, u_0)) + \tilde{R}_{u,f}^n,
\end{aligned} \tag{2.31}$$

where the truncation error  $\tilde{R}_{u,f}^n$  satisfies

$$\tilde{R}_{u,f}^n = O(h^2 t_n^{\delta_{\tilde{m}_f+1}-2}) + O(h^2 t_n^{\sigma_{\tilde{m}_u+1}-2}). \tag{2.32}$$

Inserting (2.31) into (2.18) leads to

$$\begin{aligned}
u(t_n) &= u_0 + \lambda I_{h,\sigma}^{\beta,n,m_u} u + I_{h,\delta}^{\beta,n,m_f} f_u \\
&\quad + h^\beta \omega_0^{(\beta)} \left[ -f(t_n, u(t_n)) + f(t_{n-1}, u(t_{n-1})) + h \partial_t f(t_{n-1}, u(t_{n-1})) \right. \\
&\quad + \partial_u f(t_{n-1}, u(t_{n-1})) \left( u(t_n) - u(t_{n-1}) + \sum_{k=1}^{\tilde{m}_u} \widetilde{W}_{n,k}^{(u)} (u(t_k) - u_0) \right) \\
&\quad \left. + \sum_{k=1}^{\tilde{m}_f} \widetilde{W}_{n,k}^{(f)} (f(t_k, u(t_k)) - f(t_0, u_0)) \right] + R_T^n,
\end{aligned} \tag{2.33}$$

where  $R_T^n = R_u^n + R_f^n + h^\beta \tilde{R}_{u,f}^n$ ,  $R_u^n$ ,  $R_f^n$ , and  $\tilde{R}_{u,f}^n$  are defined by (2.13), (2.17), and (2.32), respectively.

From (2.33), we obtain the IMEX method based on the Taylor expansion technique (abbreviated as **IMEX-T**) as: given  $U_k (0 \leq k \leq n-1)$ , to find  $U_n (n \geq 2)$  such that

$$\begin{aligned} U_n = & U_0 + \lambda I_{h,\sigma}^{\beta,n,m_u} U + I_{h,\delta}^{\beta,n,m_f} F + h^\beta \omega_0^{(\beta)} \left[ -F_n + F_{n-1} + h \partial_t f(t_{n-1}, U_{n-1}) \right. \\ & \left. + \partial_u f(t_{n-1}, U_{n-1}) \left( U_n - U_{n-1} + \sum_{k=1}^{\tilde{m}_u} \widetilde{W}_{n,k}^{(u)} (U_k - U_0) \right) + \sum_{k=1}^{\tilde{m}_f} \widetilde{W}_{n,k}^{(f)} (F_k - F_0) \right], \end{aligned} \quad (2.34)$$

where  $F_k = f(t_k, U_k)$ ,  $\omega_0^{(\beta)} = 2^{-\beta}$ ,  $I_{h,\sigma}^{\beta,n,m_u}$  and  $I_{h,\delta}^{\beta,n,m_f}$  are defined by (2.9),  $\widetilde{W}_{n,k}^{(f)}$  and  $\widetilde{W}_{n,k}^{(u)}$  are given by (2.28) and (2.30), respectively.

Next, we present the convergence results for the two schemes (2.26) and (2.34), the proofs of which will be given in Section 6.

**Theorem 2.5 (Convergence of IMEX-E)** *Suppose that  $u(t)$  is the solution to (2.1) that satisfies (2.8) and  $U_n$  is the solution to (2.26), and  $f(t, u)$  satisfies the Lipschitz condition with respect to the second argument  $u$ . If  $\sigma_{m_u}, \delta_{m_f} \leq 2$  and  $\delta_{\tilde{m}_f} \leq 2 + \beta$ , then there exists a positive constant  $C$  independent of  $h$  and  $n$  such that*

$$|u(t_n) - U_n| \leq C \left( \sum_{k=1}^m |u(t_k) - U_k| + h^q \right), \quad (2.35)$$

where  $m = \max\{m_u, m_f, \tilde{m}_f\}$  and  $q = \min\{2, \sigma_{m_u+1} + \beta, \delta_{m_f+1} + \beta, \delta_{\tilde{m}_f+1} + \beta\}$ .

**Theorem 2.6 (Convergence of IMEX-T)** *Suppose that  $u(t)$  is the solution to (2.1) that satisfies (2.8) and  $U_n$  is the solution to (2.34), and  $f(t, u)$  satisfies the Lipschitz condition with respect to the second argument  $u$ . If  $\sigma_{m_u}, \delta_{m_f} \leq 2$  and  $\sigma_{\tilde{m}_u}, \delta_{\tilde{m}_f} \leq 2 + \beta$ , then there exists a positive constant  $C$  independent of  $h$  and  $n$  such that*

$$|u(t_n) - U_n| \leq C \left( \sum_{k=1}^m |u(t_k) - U_k| + h^q \right), \quad (2.36)$$

where  $m = \max\{m_u, m_f, \tilde{m}_f, \tilde{m}_u\}$  and

$$q = \min\{2, \sigma_{m_u+1} + \beta, \delta_{m_f+1} + \beta, \delta_{\tilde{m}_f+1} + \beta, \sigma_{\tilde{m}_u+1} + \beta\}.$$

### 3 Linear stability of IMEX schemes

In this section, we discuss the linear stability of the proposed IMEX schemes for the scalar equation

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

We recall the definition of stability for the linear equation (3.1).

**Theorem 3.1 ([29, 30])** *Let  $\beta > 0$ . The steady-state solution  $u = 0$  of Eq. (3.1) is stable if and only if  $(\lambda + \rho) \in \sum_\beta$ , where  $\sum_\beta = \{s \in \mathbb{C} : |\arg(s)| > \frac{\beta\pi}{2}\}$ .*

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

The following theorem is useful to determine stability regions of the numerical schemes.



**Theorem 3.3** ([17, 18, 31]) *Let  $\beta > 0$ . Assume that the sequence  $\{g_n\}$  is convergent and that the quadrature weights  $w_n$  ( $n \geq 1$ ) satisfy*

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

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

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

*where  $\xi = \lambda h^{\beta}$  or  $\xi$  is some function of  $\lambda h^{\beta}$ .*

We first consider the linear stability of the IMEX-E scheme for the test equation (3.1). From the IMEX-E scheme (2.26), we get

$$\begin{aligned} U_n &= U_0 + (\lambda + \rho) h^{\beta} \left[ \sum_{k=0}^n \omega_{n-k}^{(\beta)} U_k + \sum_{k=1}^{m_u} W_{n,k}^{(\beta, \sigma)} U_k + B_n^{\sigma} U_0 \right] \\ &\quad + \rho h^{\beta} \omega_0^{(\beta)} \left[ -U_n + 2U_{n-1} - U_{n-2} + \sum_{k=1}^{\tilde{m}_f} \widehat{W}_{n,k}^{(f)} (U_k - U_0) \right] \\ &= U_0 + (\lambda + \rho) h^{\beta} \sum_{k=0}^n \omega_{n-k}^{(\beta)} U_k - \rho h^{\beta} \omega_0^{(\beta)} (U_n - 2U_{n-1} + U_{n-2}) + h^{\beta} \sum_{k=0}^m \omega_{n,k} U_k, \end{aligned} \quad (3.3)$$

where  $\sum_{k=0}^m \omega_{n,k} U_k = (\lambda + \rho) \sum_{k=1}^{m_u} W_{n,k}^{(\beta, \sigma)} U_k + B_n^{\sigma} U_0 + \rho \omega_0^{(\beta)} \sum_{k=1}^{\tilde{m}_f} \widehat{W}_{n,k}^{(f)} (U_k - U_0)$ . By comparing coefficients on both sides of the above identity, we can get  $\omega_{n,k}$ . Here we do not give the exact expression of  $\omega_{n,k}$ , since it does not affect the stability analysis.

Denote  $U(z) = \sum_{k=0}^{\infty} U_k z^k$ ,  $|z| \leq 1$ ,  $m_0 = \max\{m_u, \tilde{m}_f\}$ . Then we have from (3.3) that

$$\begin{aligned} \sum_{n=2}^{\infty} U_n z^n &= U_0 \sum_{n=2}^{\infty} z^n + (\lambda + \rho) h^{\beta} \sum_{n=2}^{\infty} \left( \sum_{k=0}^n \omega_{n-k}^{(\beta)} U_k \right) z^n \\ &\quad - \rho h^{\beta} \omega_0^{(\beta)} \sum_{n=2}^{\infty} (U_n - 2U_{n-1} + U_{n-2}) z^n + h^{\beta} \sum_{k=0}^{m_0} U_k \left( \sum_{n=2}^{\infty} \omega_{n,k} z^n \right), \end{aligned}$$

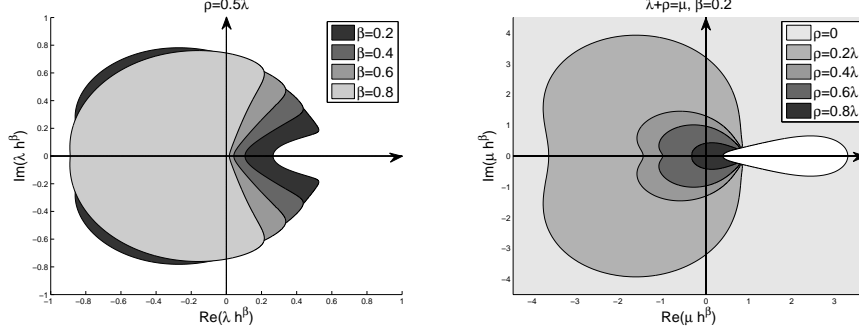
which leads to

$$\begin{aligned} U(z) - U_0 - U_1 z &= U_0 (1 - z)^{-1} - U_0 (1 + z) \\ &\quad + (\lambda + \rho) h^{\beta} \left( U(z) \omega^{(\beta)}(z) - \omega_0^{(\beta)} U_0 - (\omega_0^{(\beta)} U_1 + \omega_1^{(\beta)} U_0) z \right) \\ &\quad - \rho h^{\beta} \omega_0^{(\beta)} \left( (1 - z)^2 U(z) - (1 - 2z) U_0 - U_1 z \right) + h^{\beta} \sum_{k=0}^{m_0} \tilde{\omega}_k(z) U_k, \end{aligned} \quad (3.4)$$

where  $\tilde{\omega}_k(z) = \sum_{n=2}^{\infty} \omega_{n,k} z^n$ . We simplify (3.4) as

$$\left( 1 - (\lambda + \rho) h^{\beta} \omega^{(\beta)}(z) + \rho h^{\beta} \omega_0^{(\beta)} (1 - z)^2 \right) U(z) = H(z) = \sum_{n=0}^{\infty} H_n z^n, \quad (3.5)$$

Figure 1: Stability region of the IMEX-E scheme (shaded) for the test equation (3.1); left: stability region varying with different  $\beta$  and  $\rho = 0.5\lambda$ ; right: stability region varying with different  $\rho$  restricted to  $\lambda + \rho = \mu$ , and  $\beta = 0.2$ .



where  $H(z) = U_0(1-z)^{-1} + (U_1 - U_0)z - (\lambda + \rho)h^\beta \left( \omega_0^{(\beta)}U_0 + (\omega_0^{(\beta)}U_1 + \omega_1^{(\beta)}U_0)z \right) + \rho h^\beta \omega_0^{(\beta)}((1-2z)U_0 + U_1z) + h^\beta \sum_{k=0}^{m_0} \tilde{\omega}_k(z)U_k$ .

It is readily verified that  $\{H_n\}$  is a convergent sequence if  $\sigma_{m_u}, \delta_{\tilde{m}_f} \leq 2 - \beta$ ; see Lemmas 6.1 and 6.2. From Theorem 3.3, we obtain that the scheme (2.26) is stable if

$$1 - (\lambda + \rho)h^\beta \omega^{(\beta)}(z) + \rho h^\beta \omega_0^{(\beta)}(1-z)^2 \neq 0, \quad \forall |z| \leq 1. \quad (3.6)$$

We summarize the above argument and have the following theorem.

**Theorem 3.4 (Linear stability of IMEX-E)** *Let  $\rho = k\lambda$  and  $\xi = \lambda h^\beta$ . Then the stability region of the method (2.26) for (3.1) is*

$$\Sigma_\beta^{Num} = \mathbb{C} \setminus \left\{ \xi \mid \xi = \frac{1}{(k+1)\omega^{(\beta)}(z) - k\omega_0^{(\beta)}(1-z)^2}, |z| \leq 1 \right\}, \quad (3.7)$$

Fig. 1 shows the stability region of the IMEX-E scheme with different  $\beta$  and  $\rho/\lambda$ . Moreover, if  $\lambda, \rho \in \mathbb{R}$  and  $\rho + \lambda = \text{constant}$ , i.e.,  $\rho + \lambda = -1$ , then we have  $-1 \leq \rho \leq 0$ . In such a case, we should have  $h^\beta \neq \frac{2^\beta(1-z)^\beta}{-(1+z)^\beta - \rho(1-z)^{2+\beta}}, |z| \leq 1$ . Hence, the stability condition of the method (2.26) for the model problem (3.1) with  $\lambda + \rho = -1$  satisfies

$$h^\beta \in \left( 0, -\frac{2^\beta}{4\rho} \right).$$

Clearly, the length of the stability interval decreases as  $\rho \rightarrow -1$ , which is consistent with the theoretical result of the case  $\beta = 1$ .

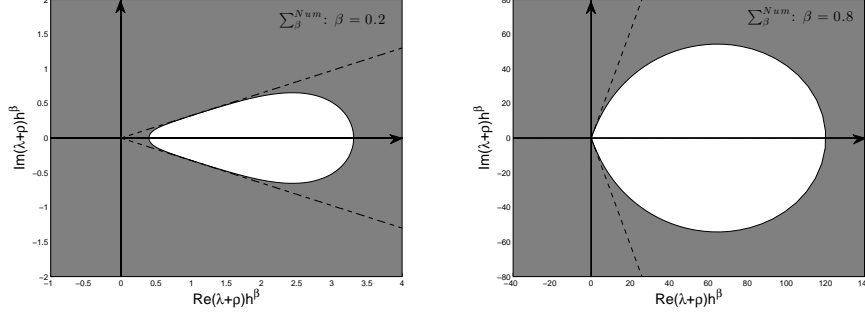
Next we consider the linear stability of the scheme IMEX-T (2.34). Applying (2.34) to (3.1) and letting  $f(t, U) = (\rho + \lambda)U$ , we have the stability region of (2.34) in the following theorem, see also [31] and Fig. 2.

**Theorem 3.5 (Linear stability of IMEX-T)** *The stability region of the method (2.34) for (3.1) is*

$$\Sigma_\beta^{Num} = \mathbb{C} \setminus \left\{ \xi \mid \xi = \frac{1}{\omega^{(\beta)}(z)}, |z| \leq 1 \right\}, \quad (3.8)$$

where  $\xi = (\lambda + \rho)h^\beta$ , and  $\omega^{(\beta)}(z)$  is defined by (2.6).

Figure 2: Stability region of the IMEX-T scheme (shaded) for the test equation (3.1); left:  $\beta = 0.2$ , right:  $\beta = 0.8$



## 4 Extensions

Besides the IMEX-E and IMEX-T schemes that we have derived, some other second-order IMEX schemes can be obtained by using different approximations of  $(I_0^\beta u)(t_n)$ .

Let  $\{\omega_j^{(\beta)}\}$  be coefficients of the Taylor expansion of the following generating function

$$\omega^{(\beta)}(z) = (1-z)^{-\beta} \left(1 - \frac{\beta}{2}(1-z)\right) = \sum_{j=0}^{\infty} \omega_j^{(\beta)} z^j, \quad (4.1)$$

$$\text{or} \quad \omega^{(\beta)}(z) = (3/2 - 2z - z^2/2)^{-\beta} = \sum_{j=0}^{\infty} \omega_j^{(\beta)} z^j. \quad (4.2)$$

Replacing the generating function (2.6) with (4.1) or (4.2) and repeating the procedures below Eq. (2.6) in Section 2 leads to new IMEX schemes, which have exactly the same form as the IMEX-E and IMEX-T schemes but using different weights.

Next, we present the trapezoidal rule [11] with correction terms that is given by

$$\begin{aligned} I_0^\beta u(t_n) &= \left[ I_0^\beta (u(t) - u(t_0)) \right]_{t=t_n} + \frac{u(t_0)t_n^\beta}{\Gamma(1+\beta)} \\ &= h^\beta \sum_{j=0}^n b_{n,j}^{(\beta)} (u(t_j) - u_0) + h^\beta \sum_{j=1}^{m_u} \widetilde{W}_{n,j}^{(\beta,\sigma)} (u(t_j) - u_0) + \frac{u_0 t_n^\beta}{\Gamma(1+\beta)} + O(h^2) \\ &= h^\beta \sum_{j=1}^n b_{n,j}^{(\beta)} u(t_j) + h^\beta \sum_{j=1}^{m_u} \widetilde{W}_{n,j}^{(\beta,\sigma)} u(t_j) + h^\beta \widetilde{B}_n^\sigma u_0 + O(h^2), \end{aligned} \quad (4.3)$$

where  $b_{n,0}^{(\beta)} = [(n-1)^{\beta+1} - (n-1-\beta)n^\beta]/\Gamma(2+\beta)$ ,  $b_{n,n}^{(\beta)} = 1/\Gamma(2+\beta)$ ,  $b_{n,j}^{(\beta)} = \frac{1}{\Gamma(2+\beta)}[(n-j+1)^{\beta+1} - 2(n-j)^{\beta+1} + (n-j-1)^{\beta+1}]$  ( $1 \leq j \leq n-1$ ), and the starting weights  $\{\widetilde{W}_{n,j}^{(\beta,\sigma)}\}$  can be derived by solving the following linear system

$$\sum_{k=1}^{m_u} \widetilde{W}_{n,k}^{(\beta,\sigma)} k^{\sigma_r} = \frac{\Gamma(\sigma_r+1)}{\Gamma(\sigma_r+1+\beta)} n^{\sigma_r+\beta} - \sum_{k=1}^n b_{n,k}^{(\beta)} k^{\sigma_r}, \quad 1 \leq r \leq m_u, \quad (4.4)$$

and  $\tilde{B}_n^\sigma$  is given by

$$\tilde{B}_n^\sigma = \frac{n^\beta}{\Gamma(1+\beta)} - \sum_{k=1}^n b_{n,k}^{(\beta)} - \sum_{k=1}^{m_u} \tilde{W}_{n,k}^{(\beta,\sigma)}.$$

Similar to deriving the IMEX-E scheme (2.34), we get the IMEX scheme for FODE (2.1) based on the extrapolation and the trapezoidal rule (abbreviated as **IMEX-E-Trap**): given  $U_k (0 \leq k \leq n-1)$ , to find  $U_n (n \geq 2)$  such that

$$\begin{aligned} U_n = & U_0 + \lambda h^\beta \left[ \sum_{k=1}^n b_{n,k}^{(\beta)} U_k + \sum_{k=1}^{m_u} \tilde{W}_{n,k}^{(\beta,\sigma)} U_k + \tilde{B}_n^\sigma U_0 \right] \\ & + h^\beta \left[ \sum_{k=1}^{n-1} b_{n,k}^{(\beta)} F_k + \sum_{k=1}^{m_f} \tilde{W}_{n,k}^{(\beta,\delta)} F_k + \tilde{B}_n^\delta F_0 \right] \\ & + h^\beta b_{n,n}^{(\beta)} \left[ 2F_{n-1} - F_{n-2} + \sum_{k=1}^{\tilde{m}_f} \widehat{W}_{n,k}^{(f)} (F_k - F_0) \right], \end{aligned} \quad (4.5)$$

where  $F_n = f(t_n, U_n)$ ,  $b_{n,k}^{(\beta)}$  is given in (4.3),  $\tilde{W}_{n,k}^{(\beta,\sigma)}$  is defined in (4.4),  $\widehat{W}_{n,k}^{(f)}$  is given by (2.23),  $\tilde{B}_n^\delta = \frac{n^\beta}{\Gamma(1+\beta)} - \sum_{k=1}^n b_{n,k}^{(\beta)} - \sum_{k=1}^{m_f} \tilde{W}_{n,k}^{(\beta,\delta)}$ , and  $\tilde{W}_{n,k}^{(\beta,\delta)}$  can be derived by solving the linear system

$$\sum_{k=1}^{m_f} \tilde{W}_{n,k}^{(\beta,\delta)} k^{\delta_r} = \frac{\Gamma(\delta_r + 1)}{\Gamma(\delta_r + 1 + \beta)} n^{\delta_r + \beta} - \sum_{k=1}^n b_{n,k}^{(\beta)} k^{\delta_r}, \quad 1 \leq r \leq m_f. \quad (4.6)$$

The Taylor expansion used in the IMEX-T scheme can be also applied here to get another IMEX scheme with the trapezoidal rule. We omit the details here due to the similarity.

The present IMEX-E and IMEX-T schemes can be extended to the following multi-term fractional ordinary differential system

$$({}^C D_0^\alpha u)(t) + ({}^C D_0^\beta u)(t) = Au(t) + f_u(t), \quad t \in (0, T], \quad u(0) = u_0, \quad (4.7)$$

where  $A$  is a real-valued matrix. Let  $\alpha < \beta$ . We can transform (4.7) into its integral form as

$$u(t) = u(0) - (I_0^{\beta-\alpha} (u - u(0)))(t) + A(I_0^\beta u)(t) + (I_0^\beta f_u)(t), \quad 0 \leq t \leq T. \quad (4.8)$$

Then we apply (2.9) to discretize each fractional integral in (4.8), and corresponding IMEX schemes similar to (2.26), (2.34) and (4.5) can be derived. For instance, the IMEX-E scheme for (4.7) reads

$$\begin{aligned} U_n = & U_0 - I_{h,\sigma}^{\beta-\alpha,n,m_u^1} (U - U_0) + A I_{h,\sigma}^{\beta,n,m_u^2} U + I_{h,\delta}^{\beta,n,m_f} F \\ & + h^\beta \omega_0^{(\beta)} \left[ -F_n + 2F_{n-1} - F_{n-2} + \sum_{k=1}^{\tilde{m}_f} \widehat{W}_{n,k}^{(f)} (F_k - F_0) \right], \end{aligned} \quad (4.9)$$

where  $I_{h,\sigma}^{\beta-\alpha,n,m_u^1}$ ,  $I_{h,\sigma}^{\beta,n,m_u^2}$  and  $I_{h,\delta}^{\beta,n,m_f}$  are defined by (2.9) and  $\widehat{W}_{n,k}^{(f)}$  is defined by (2.23). Since the IMEX-T and IMEX-Trap schemes can be also derived readily, we do not present them here.

When using uniform stepsize, the TS-I and TS-III schemes in [1] can be readily rewritten as the IMEX forms. For comparison, we present IMEX forms of the TS-I and TS-III schemes for (4.7).

**IMEX form of TS-I:**

$$\begin{aligned}
U_n &= U_0 + w_{n,n}^{(\beta-\alpha)} n^{\beta-\alpha} U_0 - \sum_{j=1}^{n-1} w_{n,j}^{(\beta-\alpha)} U_{j-\frac{1}{2}} - w_{n,n}^{(\beta-\alpha)} U_n \\
&\quad + A \left( \sum_{j=1}^{n-1} w_{n,j}^{(\beta)} U_{j-\frac{1}{2}} + w_{n,n}^{(\beta)} U_n \right) + \sum_{j=1}^{n-1} w_{n,j}^{(\beta)} f(t_{j-\frac{1}{2}}, U_{j-\frac{1}{2}}) + w_{n,n}^{(\beta)} f(t_{n-1}, U_{n-1}),
\end{aligned}$$

where  $U_{j-\frac{1}{2}} = \frac{U_{j-1}+U_j}{2}$  and  $w_{n,j}^{(\nu)} = \frac{h^\nu}{\Gamma(1+\nu)}[(n-j+1)^\nu - (n-j)^\nu]$ ,  $\nu = \beta, \beta - \alpha$ .

**IMEX form of TS-III:**

$$\begin{aligned}
&\sum_{j=1}^n b_{n,j}^{(\alpha)} (U_j - U_{j-1}) + \sum_{j=1}^n b_{n,j}^{(\beta)} (U_j - U_{j-1}) \\
&= AU_n + f(t_n, U_{n-1}) + \text{diag}[f_u(t_n, U_{n-1})](U_n - U_{n-1}),
\end{aligned}$$

where  $b_{n,j}^{(\nu)} = \frac{h^{-\nu}}{\Gamma(2-\nu)}[(n-j+1)^{1-\nu} - (n-j)^{1-\nu}]$ ,  $\nu = \alpha, \beta$ , and  $\text{diag}[\cdot]$  denotes the diagonal matrix where the  $k$ -th diagonal element is the  $k$ -th element of a vector,  $k = 1, 2, \dots, m$ .

We will test the schemes IMEX-E, IMEX-T and IMEX-E-Trap in Example 5.3 and compare the numerical results with the TS-I, TS-III schemes and the predictor-corrector scheme [10]. Convergence analysis will not be presented in this paper. However, it will be shown numerically that the IMEX-E, IMEX-T and IMEX-E-Trap schemes are of uniformly second-order accuracy for solving (5.8) with non-smooth solutions or smooth solutions.

## 5 Numerical examples

We denote by  $U_n$  a numerical solution of the numerical methods in the present work with a time step size  $h$  at  $t_n = nh$ , and we measure the errors in the following sense:

$$E_\infty^r(h) = \frac{\max_{0 \leq n \leq N} |U_n^{\text{ref}} - U_n|}{\max_{0 \leq n \leq N} |U_n^{\text{ref}}|}, \quad E_N^r(h) = \frac{|U_N^{\text{ref}} - U_N|}{|U_N^{\text{ref}}|}.$$

If the exact solution  $u(t)$  is available, then we take  $U_n^{\text{ref}} = u(t_n)$ ; otherwise we obtain the reference solution  $U_n^{\text{ref}}$  with the step size  $h = 2^{-15}$ .

We will test accuracy and convergence order of the IMEX-E and IMEX-T schemes for a stiff system and a nonlinear equation with non-smooth solutions in Examples 5.1 and 5.2, respectively. In Example 5.3, we will show the behavior of the IMEX-E, IMEX-T and IMEX-Trap schemes when solving a multi-term nonlinear stiff fractional differential system. We will also compare our methods with the TS-I, TS-III schemes proposed in [1] (see their IMEX forms in Section 4), and the predictor-corrector (PC) scheme developed in [10] for  $({}^C D_0^\beta u)(t) = f(t, u)$ ,  $t \in (0, T]$ ,  $u(0) = u_0$ :

$$u_n^p = u_0 + \sum_{j=0}^{n-1} w_{n-1,j}^{(\beta)} f(t_j, u_j), \tag{5.1}$$

$$u_n = u_0 + h^\beta b_{n,n}^{(\beta)} f(t_n, u_n^p) + h^\beta \sum_{j=0}^{n-1} b_{n,j}^{(\beta)} f(t_j, u_j), \tag{5.2}$$

where  $w_{n,j}^{(\beta)} = \frac{h^\beta}{\Gamma(1+\beta)}[(n-j+1)^\beta - (n-j)^\beta]$ , and  $b_{n,j}^{(\beta)}$  is defined in (4.3).

**Example 5.1 (Stiff fractional ordinary differential system)**

$$\begin{aligned}({}^C D_0^\beta u)(t) &= Au(t) + Bu(t) + g(t), \quad t \in (0, T], \\ u(0) &= u_0.\end{aligned}\tag{5.3}$$

In this example, we take  $f(t, u) = Bu(t) + g(t)$  and use the IMEX-E scheme (2.26) to solve this system. Take  $u_0 = (u_{01}, u_{02}, u_{03})^\top = (1, 1, 1)^\top$ ,

$$A = \begin{pmatrix} -10000 & 0 & 1 \\ -0.05 & -0.08 & -0.2 \\ 1 & 0 & -1 \end{pmatrix}, \quad B = \begin{pmatrix} -0.6 & 0 & 0.2 \\ -0.1 & -0.2 & 0 \\ 0 & -0.5 & -0.8 \end{pmatrix},\tag{5.4}$$

and

$$g(t) = \begin{pmatrix} a_1 \Gamma_1 t^{\sigma_1 - \beta} + a_2 \Gamma_2 t^{\sigma_2 - \beta} \\ a_3 \Gamma_3 t^{\sigma_3 - \beta} + a_4 \Gamma_4 t^{\sigma_4 - \beta} \\ a_5 \Gamma_5 t^{\sigma_5 - \beta} + a_6 \Gamma_6 t^{\sigma_6 - \beta} \end{pmatrix} - (A + B) \begin{pmatrix} a_1 t^{\sigma_1} + a_2 t^{\sigma_2} + u_{01} \\ a_3 t^{\sigma_3} + a_4 t^{\sigma_4} + u_{02} \\ a_5 t^{\sigma_5} + a_6 t^{\sigma_6} + u_{03} \end{pmatrix},\tag{5.5}$$

where  $\Gamma_k = \frac{\Gamma(\sigma_k + 1)}{\Gamma(\sigma_k + 1 - \beta)}$  ( $1 \leq k \leq 6$ ). Then the exact solution of (5.3) is

$$u(t) = (a_1 t^{\sigma_1} + a_2 t^{\sigma_2} + u_{01}, a_3 t^{\sigma_3} + a_4 t^{\sigma_4} + u_{02}, a_5 t^{\sigma_5} + a_6 t^{\sigma_6} + u_{03})^\top.\tag{5.6}$$

We take  $\sigma_1 = \beta$ ,  $\sigma_2 = 2\beta$ ,  $\sigma_3 = 1 + \beta$ ,  $\sigma_4 = 5\beta$ ,  $\sigma_5 = 2$ ,  $\sigma_6 = 2 + \beta$ , and  $a_1 = 0.5$ ,  $a_2 = 0.8$ ,  $a_3 = 1$ ,  $a_4 = 1$ ,  $a_5 = 1$ ,  $a_6 = 1$  in the numerical computation.

Table 1: Relative error and convergence rate of the IMEX-E scheme (2.26) with different correction terms for the stiff system (5.3) (Example 5.1),  $T = 1$ ,  $\beta = 0.1$ .

$h$	$m = 0$		$m = 1$		$m = 2$		$m = 3$		$m = 4$	
	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order
$2^{-10}$	9.45e-3	0.24	1.13e-3	0.48	1.33e-4	0.61	2.43e-6	1.19	2.27e-7	2.05
$2^{-11}$	8.02e-3	0.23	8.10e-4	0.46	8.68e-5	0.60	1.07e-6	1.17	5.46e-8	2.05
$2^{-12}$	6.83e-3	0.23	5.89e-4	0.43	5.74e-5	0.58	4.73e-7	1.16	1.32e-8	2.05
$2^{-13}$	5.83e-3	*	4.36e-4	*	3.83e-5	*	2.11e-7	*	3.17e-9	*

Table 2: Relative error and convergence rate of the IMEX-E scheme (2.26) with different correction terms for the stiff system (5.3) (Example 5.1),  $T = 1$ ,  $\beta = 0.5$ .

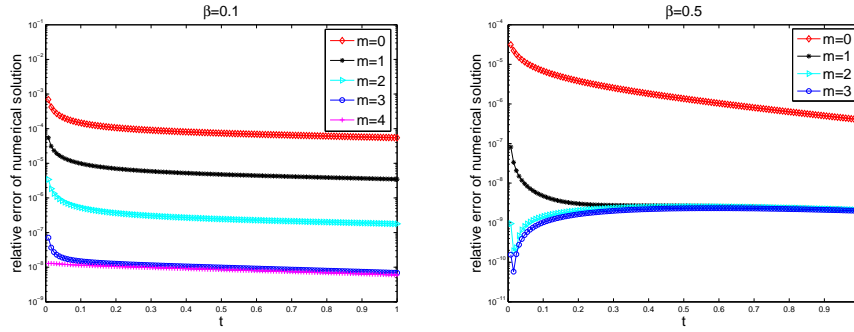
$h$	$m = 0$		$m = 1$		$m = 2$		$m = 3$	
	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order
$2^{-10}$	8.27e-4	0.50	3.71e-5	1.00	1.06e-7	2.07	2.95e-8	1.80
$2^{-11}$	5.84e-4	0.50	1.86e-5	1.00	2.52e-8	2.05	8.46e-9	1.87
$2^{-12}$	4.12e-4	0.50	9.28e-6	1.00	6.11e-9	2.03	2.32e-9	1.91
$2^{-13}$	2.91e-4	*	4.63e-6	*	1.49e-9	*	6.17e-10	*

Tables 1 and 2 show that the use of starting values in the IMEX-E scheme is crucial for both reducing relative errors and getting uniformly second-order accuracy. We observe that the fractional system (5.3) with smaller fractional order  $\beta = 0.1$  requires more correction terms than that with bigger fractional order  $\beta = 0.5$ , which is consistent with Theorem 2.5. Moreover, from the data in the last column of Table 2, we find that no gain of convergence rate is observed when the number of correction terms exceeds some optimal number that can be derived from Theorem 2.5. Specifically, the global second-order accuracy can

Table 3: Condition numbers and residuals of the linear system (2.10) (Example 5.1),  $\sigma_1 = \beta$ ,  $\sigma_2 = 2\beta$ ,  $\sigma_3 = 1 + \beta$ ,  $\sigma_4 = 5\beta$ .

$\beta$	-	$m = 2$	$m = 3$	$m = 4$
0.1	condition numbers	6.20e+01	1.70e+03	2.85e+04
	residuals	6.94e-18	5.55e-17	1.11e-15
0.5	condition numbers	1.74e+01	2.65e+02	5.11e+03
	residuals	5.54e-17	1.10e-16	8.53e-14

Figure 3: Comparison of relative errors for the IMEX-E scheme with different correction terms for the stiff system (5.3) (Example 5.1),  $h = 2^{-12}$ ,  $T = 1$ . All needed starting values are given in advance.



be obtained when  $\min\{\sigma_{m+1} + \beta, \delta_{m+1} + \beta\} \geq 2$ . For  $\beta = 0.1$ , the smallest  $m$  to get the global second-order accuracy is 4, while for  $\beta = 0.5$ , the optimal  $m$  is 2; numerical results in Tables 1–2 verify the theoretical results in Theorem 2.5. Data in the last column of Table 2 also imply that too many correction terms are not always helpful, which can be also illustrated from Lemma 6.2, where the starting weights (see, e.g.  $W_{n,k}^{(\beta,\sigma)}$  in (6.1)) will be large when  $\sigma_r$  is sufficiently large. However, from the condition numbers and residuals of (2.10) in Table 3, we observe that relatively high accuracy of starting weights can be obtained even when the condition number is large if there are only a few correction terms. Here and in Table 6, the residual is computed by

$$\max_{1 \leq r \leq m, 1 \leq n \leq 100} \left| \sum_{k=1}^m W_{n,k}^{(\beta,u)} k^{\sigma_r} - \frac{\Gamma(\sigma_r + 1)}{\Gamma(\sigma_r + 1 + \beta)} n^{\sigma_r + \beta} + \sum_{k=0}^n \omega_{n-k}^{(\beta)} k^{\sigma_r} \right|.$$

We further solve (5.3) by the predictor-corrector scheme (5.1)-(5.2) for comparison. In our tests, numerical solutions of the predictor-corrector scheme blow up very quickly for  $\beta = 0.1$  and  $\beta = 0.5$ , even if we take very small step size  $h = 2^{-16}$ . For bigger  $\beta$  (i.e.,  $\beta = 0.95$ ), the predictor-corrector scheme cannot work either, except that we take very small stepsize (i.e.,  $h = 2^{-13}$ ). We do not present all these results here.

Figure 3 shows the asymptotic behavior of relative errors for the IMEX-E scheme with different number of correction terms. It is shown that suitable correction terms can improve the accuracy greatly. Moreover, there exists an optimal number of correction terms for both  $\beta = 0.1$  and  $\beta = 0.5$ . If one applies more correction terms than the optimal choice, the accuracy may not be further improved. In this example, all necessary starting values have been given in advance (We have analytical solutions). However, in practice, we have to calculate starting values numerically using high-order methods or using small stepsizes, which will be shown in the following example.

Table 4: Relative error and convergence rate of the IMEX-T scheme (2.34) for the nonlinear equation (5.7) (Example 5.2, Case I),  $T = 8$ ,  $\beta = 0.15$ .

$h$	$m = 0$		$m = 1$		$m = 2$		$m = 3$		$m = 4$	
	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order	$E_\infty^r(h)$	order
$2^{-5}$	8.99e-4	0.11	6.05e-4	0.94	1.07e-3	1.71	6.20e-4	2.07	6.04e-4	2.04
$2^{-6}$	9.70e-4	0.30	3.14e-4	0.08	3.27e-4	1.36	1.46e-4	2.01	1.46e-4	2.10
$2^{-7}$	7.87e-4	0.38	2.95e-4	0.37	1.27e-4	1.02	3.64e-5	1.77	3.40e-5	2.13
$2^{-8}$	6.03e-4	0.39	2.28e-4	0.43	6.26e-5	0.81	1.06e-5	1.45	7.76e-6	2.14
$2^{-9}$	4.59e-4	*	1.68e-4	*	3.56e-5	*	3.88e-6	*	1.76e-6	*

**Example 5.2 (Nonlinear fractional ordinary differential equation)**

$$({}^C D_0^\beta u)(t) = \lambda u(t) + \rho u(1 - u^2) + g(t), t \in (0, T], \quad u(0) = u_0. \quad (5.7)$$

- Case I: Take  $\lambda = -3$ ,  $\rho = 0.8$ . Choose suitable  $g(t)$  such that the solution to (5.7) is  $u(t) = u_0 + \sum_{k=1}^6 t^{\sigma_k}$ , where  $u_0 = 2$ ,  $\sigma_k = k\beta$  ( $1 \leq k \leq 5$ ) and  $\sigma_6 = 2 + \beta$ .
- Case II: Take  $g(t) = 0$ ,  $\lambda = -3$ ,  $\rho = 0.8$ , and  $u_0 = 2$ . From Lemma 2.1, we know that the analytical solution  $u(t)$  satisfies (2.4). So  $\sigma_k$  in (2.8) satisfies  $\sigma_k \in \{i + j\beta, i = 0, 1, \dots, j = 1, 2, \dots\}$ .

As we do not have an exact solution for Case II, we calculate a reference solution by the considered scheme with very small step size  $h = 2^{-15}$ .

Table 4 shows the maximum relative errors of the IMEX-T scheme (2.34) with different time stepsizes for solving the nonlinear equation (5.7) (Case I) when  $\beta = 0.15$ . We also apply the IMEX-E scheme (2.26) to this problem, and observe that numerical solutions blow up even for the small step size  $h = 2^{-14}$  (results not presented here).

Table 5 and Figure 4 show the relative errors and convergence rates of the IMEX-E and IMEX-T scheme for solving the nonlinear equation (5.7) (Case II). It is shown that we can apply proper correction terms for both schemes to improve their convergence order up to second-order though we do not know what the exact solution is. Here we use the adaptive step size  $h^2$  to calculate starting values of correction terms in our schemes for different stepsize  $h$ . Numerical tests show that it works well. In Table 6, we also present the condition numbers and residuals of system (2.10) for different number of correction terms.

When using the predictor-corrector scheme (5.1)-(5.2) to solve (5.7) (Case II) in this example, the numerical solution blows up for  $\beta = 0.15$  and is of convergence order  $\beta$  for  $\beta = 0.95$ ; see Table 7.

**Example 5.3 (A comparison of IMEX-T, IMEX-E, IMEX-E-Trap and TS-I, TS-III in [1], PC scheme in [10])**

In this example, we solve the following multi-term nonlinear stiff fractional differential system:

$$({}^C D_0^\alpha u)(t) + ({}^C D_0^\beta u)(t) = Au(t) + B \sin u + g(t), t \in (0, T], \quad u(0) = u_0, \quad (5.8)$$

where  $\beta = 0.55$ ,  $\alpha = 0.4$ ,

$$A = \begin{pmatrix} -1000 & 100 \\ 0 & -0.1 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}.$$

We choose suitable  $g(t)$  such that the above system has

$$\text{Case I: } u(t) = \begin{bmatrix} t^{0.55} + t^{1.15} + 1 \\ t^{0.9} + t^{2.55} + 1 \end{bmatrix}; \quad \text{Case II: } u(t) = \begin{bmatrix} t^{2.55} + t^{2.15} + 1 \\ t^3 + t^{2.55} + 1 \end{bmatrix}.$$



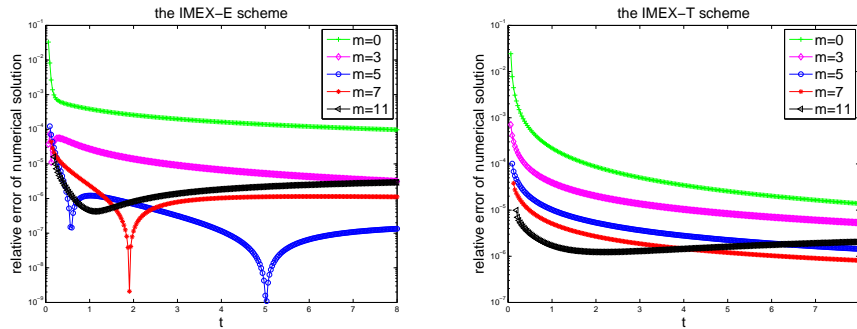
Table 5: Relative errors and convergence rate of the IMEX-E scheme (2.26) and the IMEX-T scheme (2.34). Comparison of the schemes with different correction terms for the nonlinear equation (5.7) (Example 5.2, Case II),  $T = 8$ ,  $\beta = 0.15$ .

$m$	$h$	IMEX-E			IMEX-T		
		$E_{\infty}^r(h)$	order	cputime	$E_{\infty}^r(h)$	order	cpu time
0	$2^{-4}$	2.82e-01	0.10	0.02	1.51e-01	0.21	0.03
	$2^{-5}$	2.63e-01	0.10	0.08	1.31e-01	0.21	0.05
	$2^{-6}$	2.46e-01	0.09	0.13	1.13e-01	0.21	0.13
	$2^{-7}$	2.31e-01	*	0.27	9.82e-02	*	0.28
3	$2^{-4}$	1.28e-03	1.80	0.03	2.02e-03	1.01	0.03
	$2^{-5}$	3.68e-04	0.94	0.05	1.00e-03	0.51	0.08
	$2^{-6}$	1.92e-04	0.16	0.12	7.06e-04	0.37	0.14
	$2^{-7}$	1.72e-04	*	0.29	5.48e-04	*	0.29
5	$2^{-4}$	8.23e-04	1.26	0.03	8.52e-04	1.68	0.03
	$2^{-5}$	3.45e-04	0.93	0.08	2.67e-04	1.39	0.07
	$2^{-6}$	1.81e-04	0.60	0.14	1.01e-04	1.05	0.16
	$2^{-7}$	1.20e-04	*	0.35	4.91e-05	*	0.36
7	$2^{-4}$	6.07e-04	1.58	0.06	5.83e-04	1.79	0.04
	$2^{-5}$	2.03e-04	1.60	0.07	1.68e-04	2.14	0.08
	$2^{-6}$	6.71e-05	1.40	0.16	3.81e-05	2.74	0.16
	$2^{-7}$	2.55e-05	*	0.44	5.70e-06	*	0.38
11	$2^{-4}$	3.57e-04	1.96	0.05	3.55e-04	2.05	0.06
	$2^{-5}$	9.20e-05	1.86	0.09	8.56e-05	2.45	0.09
	$2^{-6}$	2.53e-05	1.99	0.24	1.57e-05	2.10	0.22
	$2^{-7}$	6.36e-06	*	0.55	3.66e-06	*	0.64

Table 6: Condition numbers and residuals of the linear system (2.10) (Example 5.2, Case II),  $\beta = 0.15$ ,  $\sigma_k = k\beta$ ,  $k \geq 1$ .

$m$	$m = 3$	$m = 5$	$m = 7$	$m = 11$
condition numbers	2.06e+03	3.32e+06	6.43e+09	2.54e+16
residuals	5.55e-17	4.88e-15	6.81e-13	6.74e-08

Figure 4: Asymptotic relative error for the IMEX-E scheme (2.26) and IMEX-T scheme (2.34) with different correction terms for the nonlinear equation (5.7) (Example 5.2, Case II),  $T = 8$ ,  $\beta = 0.15$ .

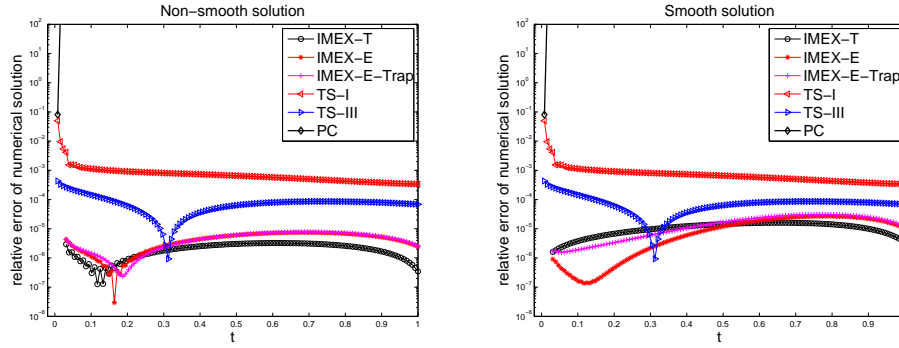


Data in Table 8 show that the IMEX-T, IMEX-E and IMEX-E-Trap schemes work well for solving the problem (5.8), with both non-smooth solution and smooth solution, obtaining second-order accuracy numerical

Table 7: Error and convergence order of the predictor-corrector scheme (5.1)–(5.2) at  $t = 8$  for the nonlinear equation (5.7) (Example 5.2, Case II).

$h$	$\beta = 0.15$	$h$	$\beta = 0.55$			$\beta = 0.95$		
	$E_N^r(h)$		$E_N^r(h)$	order	cpu time	$E_N^r(h)$	order	cpu time
$2^{-12}$	Calculation Failed	$2^{-5}$	1.62e-01	0.87	0.05	2.50e-03	1.18	0.05
$2^{-13}$	Calculation Failed	$2^{-6}$	8.86e-02	0.86	0.13	1.10e-03	1.04	0.14
$2^{-14}$	Calculation Failed	$2^{-7}$	4.87e-02	0.81	0.38	5.38e-04	0.98	0.39
$2^{-15}$	Calculation Failed	$2^{-8}$	2.78e-02	*	2.04	2.72e-04	*	2.09

Figure 5: A comparison of asymptotic behavior of relative errors of the IMEX-T, IMEX-E, IMEX-E-Trap, TS-I, TS-III, and PC schemes for the multi-term nonlinear stiff system (5.8) (Example 5.3),  $T = 1$ ,  $h = 2^{-8}$ .



solutions. It is also shown that the TS-I and TS-III schemes solve the problem (5.8) with smooth solution and get numerical solutions being of  $1 + \beta$  and  $2 - \beta$  order accuracy respectively, while for the non-smooth case, the accuracy is low and the convergence order of the TS-I and TS-III schemes is just  $\beta$ . It is worth to mention that in order to keep the uniformly second-order accuracy, we have applied suitable correction terms ( $m_u = \tilde{m}_u = 3$ ,  $m_f = \tilde{m}_f = 6$ ) in the IMEX-E, IMEX-T and IMEX-E-Trap schemes when solving the non-smooth case, and hence the CPU time of these schemes is slightly longer than that of the TS-I and TS-III schemes without correction terms with the same step size. However, to reach the same accuracy, the first three schemes are running faster than the TS-I and TS-III schemes for both non-smooth and smooth cases. In addition, neither the stiff problem (5.8) with non-smooth solution nor with smooth solution can be solved by the predictor-corrector scheme. Figure 5 shows the asymptotic relative error of all schemes for both non-smooth case and smooth case, which illustrates that the IMEX-T, IMEX-E and IMEX-E-Trap schemes are superior for solving the multi-term nonlinear stiff problem (5.8) with smooth and non-smooth solutions, compared to the TS-I scheme, TS-III scheme and the predictor-corrector scheme. We observe that numerical solutions produced by the predictor-corrector scheme blow up in this example, which confirms that the IMEX schemes we present have better stability compared to the explicit schemes. For more information on the linear stability of the predictor-corrector scheme, see [17].

## 6 Proofs

In this section, we provide the convergence analysis of the two methods (2.26) and (2.34). We first introduce two lemmas.

Table 8: A comparison of relative errors and convergence rates of the IMEX-T, IMEX-E, IMEX-E-Trap, TS-I, TS-III and PC schemes for multiterm nonlinear stiff system (5.8) with non-smooth solution (Case I) and smooth solution (Case II) (Example 5.3),  $T = 1$ .

scheme	$h$	Non-smooth solution (Case I)			Smooth solution (Case II)		
		$E_\infty^r(h)$	order	cpu time	$E_\infty^r(h)$	order	cpu time
IMEX-T	$2^{-5}$	1.30e-04	2.56	0.05	3.84e-04	2.31	0.03
	$2^{-6}$	2.19e-05	2.75	0.07	7.73e-05	2.27	0.06
	$2^{-7}$	3.25e-06	2.11	0.13	1.61e-05	2.20	0.11
	$2^{-8}$	7.51e-07	*	0.31	3.49e-06	*	0.26
IMEX-E	$2^{-5}$	2.05e-04	2.40	0.06	7.52e-04	2.40	0.04
	$2^{-6}$	3.89e-05	2.39	0.08	1.42e-04	2.40	0.07
	$2^{-7}$	7.44e-06	2.35	0.16	2.69e-05	2.38	0.14
	$2^{-8}$	1.46e-06	*	0.32	5.18e-06	*	0.30
IMEX-E-Trap	$2^{-5}$	2.11e-04	2.40	0.05	8.36e-04	2.38	0.03
	$2^{-6}$	4.02e-05	2.37	0.07	1.61e-04	2.37	0.06
	$2^{-7}$	7.79e-06	2.32	0.16	3.10e-05	2.35	0.14
	$2^{-8}$	1.56e-06	*	0.29	6.10e-06	*	0.26
TS-I	$2^{-5}$	1.10e-01	0.57	0.05	1.42e-02	1.49	0.05
	$2^{-6}$	7.39e-02	0.57	0.06	5.05e-03	1.49	0.05
	$2^{-7}$	4.97e-02	0.57	0.13	1.80e-03	1.48	0.11
	$2^{-8}$	3.35e-02	*	0.25	6.46e-04	*	0.23
TS-III	$2^{-5}$	1.10e-03	0.67	0.01	3.27e-03	1.54	0.01
	$2^{-6}$	6.93e-04	0.68	0.04	1.12e-03	1.52	0.03
	$2^{-7}$	4.31e-04	0.54	0.05	3.91e-04	1.51	0.04
	$2^{-8}$	2.97e-04	*	0.07	1.37e-04	*	0.08
PC	$2^{-5}$	Calculation	Failed		Calculation	Failed	
	$2^{-6}$	Calculation	Failed		Calculation	Failed	
	$2^{-7}$	Calculation	Failed		Calculation	Failed	
	$2^{-8}$	Calculation	Failed		Calculation	Failed	

**Lemma 6.1** ([30, 48]) *Let  $\{\omega_n^{(\beta)}\}$  be given by (2.6). Then we have  $\omega_n^{(\beta)} > 0$ , and  $\omega_n^{(\beta)} = O(n^{\beta-1})$ ,  $n > 0$ .*

**Lemma 6.2** *Let  $m_u$  and  $m_f$  be positive integers and the discrete operators  $I_{h,\sigma}^{\beta,n,m_u}$  and  $I_{h,\delta}^{\beta,n,m_f}$  be defined by (2.9). Suppose that  $\{\sigma_r\}$  and  $\{\delta_r\}$  are sequences of strictly increasing positive numbers. Then there exists a positive constant  $C$  independent of  $n$  such that*

$$|W_{n,k}^{(\beta,\sigma)}| \leq C(n^{\sigma_{m_u}+\beta-2} + n^{\beta-1}), \quad |W_{n,k}^{(\beta,\delta)}| \leq C(n^{\delta_{m_f}+\beta-2} + n^{\beta-1}). \quad (6.1)$$

**Proof.** Letting  $\nu = \sigma_r$  in (2.7), we derive

$$\frac{\Gamma(\sigma_r + 1)}{\Gamma(\sigma_r + 1 + \beta)} t_n^{\sigma_r + \beta} - h^\beta \sum_{k=0}^n \omega_{n-k}^{(\beta)} t_k^{\sigma_r} = O(h^2 t_n^{\sigma_r + \beta - 2}) + O(h^{1+\sigma_r} t_n^{\beta-1}),$$

which is equivalent to

$$\frac{\Gamma(\sigma_r + 1)}{\Gamma(\sigma_r + 1 + \beta)} n^{\sigma_r + \beta} - \sum_{k=0}^n \omega_{n-k}^{(\beta)} k^{\sigma_r} = O(n^{\sigma_r + \beta - 2}) + O(n^{\beta-1}).$$

Applying (2.10) yields

$$\sum_{k=1}^{m_u} W_{n,k}^{(\beta,\sigma)} k^{\sigma_r} = O(n^{\sigma_r + \beta - 2}) + O(n^{\beta-1}), \quad r = 1, 2, \dots, m_u,$$

which leads to  $W_{n,k}^{(\beta,\sigma)} = O(n^{\sigma_1+\beta-2}) + \dots + O(n^{\sigma_{m_u}+\beta-2}) + O(n^{\beta-1})$ . Since  $\sigma_r < \sigma_{r+1}$ , we have  $|W_{n,k}^{(\beta,\sigma)}| \leq C(n^{\sigma_{m_u}+\beta-2} + n^{\beta-1})$ . We can similarly obtain  $|W_{n,k}^{(\beta,\delta)}| \leq C(n^{\delta_{m_f}+\beta-2} + n^{\beta-1})$ , which ends the proof.  $\square$

For  $\widehat{W}_{n,k}^{(f)}$  defined by (2.23), we can easily derive

$$\sum_{k=1}^{\tilde{m}_f} \widehat{W}_{n,k}^{(f)} k^{\delta_r} = n^{\delta_r} - 2(n-1)^{\delta_r} + (n-2)^{\delta_r} = O(n^{\delta_r-2}), \quad r = 1, \dots, \tilde{m}_f,$$

which leads to

$$|\widehat{W}_{n,k}^{(f)}| \leq Cn^{\delta_{\tilde{m}_f}-2}. \quad (6.2)$$

We can similarly derive

$$|\widetilde{W}_{n,k}^{(f)}| \leq Cn^{\delta_{\tilde{m}_f}-2}, \quad |\widetilde{W}_{n,k}^{(u)}| \leq Cn^{\sigma_{\tilde{m}_u}-2}, \quad (6.3)$$

where  $\widetilde{W}_{n,k}^{(f)}$  and  $\widetilde{W}_{n,k}^{(u)}$  are defined by (2.28) and (2.30), respectively.

**Lemma 6.3 ([13])** *Let  $0 < \beta < 1$  and  $c_{n,k}$  satisfy  $0 \leq c_{n,k} \leq (n-k)^{\beta-1}$ ,  $0 \leq k \leq n$ . Assume that  $e_n$  satisfies*

$$|e_n| \leq A_0 + Mh^\beta \sum_{k=0}^{n-1} c_{n,k} |e_k|, \quad n = 1, 2, \dots, N,$$

where  $A_0, M > 0$  and  $nh \leq T$ ,  $T > 0$ . Then there exists a positive constant  $C$  independent of  $n, h$  such that

$$|e_n| \leq CA_0, \quad n = 1, 2, \dots, N.$$

Next, we present the proof for Theorem 2.5.

**Proof.** Let  $e_n = u(t_n) - U_n$ . Then from (2.25) and (2.26), we have the following error equation

$$\begin{aligned} e_n &= \lambda h^\beta \left[ \sum_{k=0}^n \omega_{n-k}^{(\beta)} e_k + \sum_{k=1}^{m_u} W_{n,k}^{(\beta,\sigma)} e_k \right] \\ &\quad + h^\beta \left[ \sum_{k=0}^{n-1} \omega_{n-k}^{(\beta)} (f(t_k, u(t_k)) - f(t_k, U_k)) + \sum_{k=1}^{m_f} W_{n,k}^{(\beta,\delta)} (f(t_k, u(t_k)) - f(t_k, U_k)) \right] \\ &\quad + h^\beta \omega_0^{(\beta)} \left[ 2(f(t_{n-1}, u(t_{n-1})) - f(t_{n-1}, U_{n-1})) - (f(t_{n-2}, u(t_{n-2})) - f(t_{n-2}, U_{n-2})) \right] \\ &\quad + \sum_{k=1}^{\tilde{m}_f} \widehat{W}_{n,k}^{(f)} (f(t_k, u(t_k)) - f(t_k, U_k)) \Big] + R_E^n, \end{aligned} \quad (6.4)$$

where  $R_E^n$  is defined in (2.25). By simple calculation, we can derive

$$|R_E^n| \leq Ch^q, \quad q = \min\{2, \sigma_{m_u} + 1 + \beta, \delta_{m_f} + 1 + \beta, \delta_{\tilde{m}_f} + 1 + \beta\}.$$

Since  $f(t, u)$  satisfies the Lipschitz condition with respect to the second argument  $u$ , i.e.,  $|f(t, x) - f(t, y)| \leq L|x - y|$ ,  $L > 0$ , we have from (6.4) that

$$\begin{aligned}
|e_n| &\leq |\lambda| h^\beta \left[ \sum_{k=0}^n \omega_{n-k}^{(\beta)} |e_k| + \sum_{k=1}^{m_u} |W_{n,k}^{(\beta, \sigma)}| |e_k| \right] + L h^\beta \left[ \sum_{k=0}^{n-1} \omega_{n-k}^{(\beta)} |e_k| + \sum_{k=1}^{m_f} |W_{n,k}^{(\beta, \delta)}| |e_k| \right] \\
&\quad + L h^\beta \omega_0^{(\beta)} \left[ 2|e_{n-1}| + |e_{n-2}| + \sum_{k=1}^{\tilde{m}_f} |\widehat{W}_{n,k}^{(f)}| |e_k| \right] + |R_E^n| \\
&\leq |\lambda| h^\beta \omega_0^{(\beta)} |e_n| + h^\beta \sum_{k=0}^{n-1} c_{n,k} |e_k| + h^\beta \sum_{k=1}^m W_{n,k} |e_k| + |R_E^n|,
\end{aligned} \tag{6.5}$$

where  $c_{n,k} = (|\lambda| + L) \omega_{n-k}^{(\beta)}$  ( $0 \leq k \leq n-3$ ),  $c_{n,n-2} = (|\lambda| + L) \omega_2^{(\beta)} + L \omega_0^{(\beta)}$ ,  $c_{n,n-1} = (|\lambda| + L) \omega_1^{(\beta)} + 2L \omega_0^{(\beta)}$ ,  $m = \max\{m_u, m_f, \tilde{m}_f\}$ , and  $W_{n,k} \geq 0$  satisfies

$$W_{n,k} = |\lambda| |W_{n,k}^{(\beta, \sigma)}| + L |W_{n,k}^{(\beta, \delta)}| + L \omega_0^{(\beta)} |\widehat{W}_{n,k}^{(f)}| \leq C n^\beta$$

when  $\sigma_{m_u}, \delta_{m_f} \leq 2$  and  $\delta_{\tilde{m}_f} \leq 2 + \beta$ , see Eqs. (6.1) and (6.2).

We rewrite (6.5) into the following form

$$(1 - |\lambda| \omega_0^{(\beta)} h^\beta) |e_n| \leq h^\beta \sum_{k=0}^{n-1} c_{n,k} |e_k| + h^\beta \sum_{k=1}^m W_{n,k} |e_k| + |R_E^n|. \tag{6.6}$$

Since  $\omega_n^{(\beta)} = O(n^{\beta-1})$  (see Lemma 6.1), we always have  $c_{n,k} \leq C(n-k)^{\beta-1}$ . Applying the generalized Gronwall's inequality (see Lemma 6.3), we derive

$$|e_n| \leq C \left( h^\beta \sum_{k=1}^m W_{n,k} |e_k| + |R_E^n| \right). \tag{6.7}$$

Note that  $|R_E^n| \leq C h^q$  and  $W_{n,k} \leq C n^\beta$ , we have  $h^\beta W_{n,k} \leq C t_n^\beta \leq C T^\beta$  that leads to  $|e_n| \leq C (\sum_{k=1}^m |e_k| + h^q)$ , which completes the proof.  $\square$

The proof of Theorem 2.6 is very similar, and hence it is omitted here.

## 7 Conclusion

We proposed two second-order IMEX schemes (see IMEX-E of (2.26) and IMEX-T of (2.34)) for nonlinear FODEs with non-smooth solutions by using suitable correction terms. We proved the convergence and linear stability of the IMEX-E and IMEX-T schemes. The stability region of the IMEX-E scheme is bounded, while the IMEX-T scheme is  $A(\frac{\beta\pi}{2})$ -stable, that is, the IMEX-T scheme is unconditionally stable.

In order to obtain the derived IMEX schemes, we presented the strategies of utilizing suitable correction terms both in the approximation of fractional integrals and in extrapolation or Taylor expansion which are adopted to linearize the schemes. The correction terms are useful to keep second-order accuracy of the IMEX schemes for solving nonlinear/stiff FODEs with non-smooth solutions. We further considered the extension of these strategies to construct other second-order schemes with correction terms for the considered FODEs. We also discussed how to extend the present IMEX schemes from single-term FODEs to multi-term FODEs and systems; see Section 4.

We provided numerical examples to verify the efficiency of the proposed schemes, which shows second-order convergence for both smooth and non-smooth solutions by choosing suitable correction terms when solving a stiff system, a nonlinear FODE and a stiff nonlinear multi-term fractional differential system. It was observed that when solving problems with non-smooth solution, applying suitable correction terms can significantly improve the accuracy, however, excessive use of correction terms is not conducive to raising accuracy, especially for the long-term simulation. Moreover, comparison between the present schemes and the existing ones illustrated that for the same level of accuracy, the present schemes cost less computational time for both smooth and non-smooth solutions.

In future work, we will focus on boundary value problems of fractional differential equations with non-smooth solution and propose high-order numerical methods.

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