Efficient and arbitrary high order finite difference schemes for the fractional differential equations

Peng Ding
Joint with Prof. Zhiping Mao

School of Mathematical Sciences Xiamen University

August 6, 2024

Outline

Fractional ODEs

Consider

$$\begin{aligned} &\frac{d^\alpha \phi}{dt^\alpha} = F(t, \phi(t)), \quad t > 0, \\ &\phi(0) = \phi_0, \end{aligned} \tag{1}$$

where $\frac{d^\alpha \phi}{dt^\alpha}$ is the Caputo fractional derivative of order $\alpha \in (0, 1]$ defined by

$$\frac{d^\alpha \phi}{dt^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{1}{(t-\tau)^\alpha} \frac{d\phi(\tau)}{d\tau} d\tau,$$

where $\phi(t)$, $\phi_0 \in \mathbb{R}^N$ and $F : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$.Assume that F is continuous, bounded and fulfills a Lipschitz condition with respect to the second variable such that the problem (1) is well-posed.[Diethelm and Ford,2002]

Existing works

- Finite difference methods:[Sun and Wu,2006:Lin,Li and Xu,2011;Cao and Xu,2013;Gao,Sun and Zhang,2014;Du,Yan and Liang,2018;......].
- Spectral methods:[Li and Xu,2011;Zayernouri and Karniadakis,2013;Chen, Wang and Shen,2016].
- Singularity
  correction:[Jin,Lazarov and Zhou,2016;Jin,Li and Zhou,2017;Yan, Khan and Ford,2018,2019,......]
  nonuniform meshes:[Stynes,Riordan and Gracia,2017;Mustapha,2020,......]
- Non-locality
  The inverse Laplace transform of convolution kernel:[Lubich,2002,2006,computational costs:$O(N_t log(N_t))$, storage:$O(log(N_t))$]

Existing works

- Non-locality
  Based on the following formula
$$\frac{t^{\alpha-1}}{\Gamma(\alpha)} = \frac{sin(\alpha\pi)}{\pi} \int_0^\infty s^{-\alpha} e^{-ts} ds,$$
  fast algorithms [Jiang, Zhang and Zhang,2017(computational costs:$O(N_t N_\varepsilon)$, storage:$O(N_\varepsilon)$);Yan,Sun and Zhang ,2017;Zeng,Turner and Burrage,2018;Guo, Zeng, Turner and Karniadakis,2019,......]
  The accelerated SDC: Chen,Mao and Karniadakis,2022.
- Long time simulation
  Fractional Phase filed/phase filed crystal :[Du,Yang and Zhou,2020; Tang,Yu and Zhou,2019;Mark and Mao,2017,2019,......]

Equivalence

- Applying the fractional integral to (1) yields the analytic solution

$$\begin{aligned}\phi(t) &= \phi(0) + \int_0^t \frac{(t-\tau)^{\alpha-1}}{\Gamma(\alpha)} F(\tau,\phi(\tau))d\tau \\ &= \phi_0 + \int_0^t g_\alpha(t-\tau)F(\tau,\phi(\tau))d\tau.\end{aligned} \tag{2}$$

- By the definition of gamma function and the change of integral variable, we have

$$\begin{aligned}g_\alpha(t) = \frac{t^{\alpha-1}}{\Gamma(\alpha)} &= \frac{t^{\alpha-1}}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty s^{-\alpha}e^{-s}ds \\ &= \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^\infty m^{-\alpha}e^{-mt}dm(s=mt) \\ &= \frac{1}{\Gamma(1-\alpha)\Gamma(\alpha)}\int_0^1 c_1(\theta)^{-\alpha}e^{-c_1(\theta)t}c_0(\theta)^2 d\theta(c_1(\theta)=m) \\ &= \int_0^1 c_0(\theta)e^{-c_1(\theta)t}\omega_\alpha(\theta)d\theta,\end{aligned} \tag{3}$$

Equivalence

where

$$c_1(\theta) = \frac{\theta}{1-\theta}, \quad c_0(\theta) = \frac{1}{1-\theta}, \quad \omega_\alpha(\theta) = \frac{\theta^{-\alpha}(1-\theta)^{\alpha-1}}{\Gamma(1-\alpha)\Gamma(\alpha)}. \tag{4}$$

- The substitution of (3) into (2), thanks to the fact $\int_0^1 \omega_\alpha(\theta)d\theta = 1$, we obtain

$$\begin{aligned} \phi(t) &= \phi_0 + \int_0^t g_\alpha(t-\tau)F(\tau,\phi(\tau))d\tau \\ &= \int_0^1 \left[\phi_0 + c_0(\theta)\int_0^t e^{-c_1(\theta)(t-\tau)}F(\tau,\phi(\tau))d\tau\right]\omega_\alpha(\theta)d\theta. \end{aligned} \tag{5}$$

- Define the function

$$\varphi(t,\theta) = \phi_0 + c_0(\theta)\int_0^t e^{-c_1(\theta)(t-\tau)}F(\tau,\phi(\tau))d\tau. \tag{6}$$

Equivalence

- Consequently, we get from the above two equations that the solution of the FDE (1) is given by

$$\phi(t) = \int_0^1 \varphi(t,\theta)\omega_\alpha(\theta)d\theta := \mathcal{C}[\varphi](t). \tag{7}$$

- Observe that the function $\varphi(t,\theta)$ is the solution of the following parameterized integer ordinary differential equation:

$$\begin{aligned}&\frac{\partial\varphi(t,\theta)}{\partial t} + c_1(\theta)\varphi(t,\theta) = c_0(\theta)F(t,\mathcal{C}[\varphi](t)) + c_1(\theta)\phi_0, \theta \in [0,1],\\ &\varphi(0,\theta) = \phi_0, \theta \in [0,1].\end{aligned} \tag{8}$$

- We call the above equation the *Extended Integer Differential Equation* (EIDE). Once we solve the above integer equation, the solution of the corresponding FDE can be computed immediately by using the equation (7).

Stability

Theorem (Stability)

For $0 < t \le T$*, if* $F(t,\phi)\phi \le L|\phi|$*, where* L *is a positive constant, then there exists a constant* $\epsilon > 0$ *such that the following estimate holds*

$$\|\varphi\|^2_{L^\infty[(0,T),L^2_{\omega_{\alpha,0}}(0,1)]} + \|\varphi\|^2_{L^2[(0,T),L^2_{\omega_\alpha}(0,1)]} \le C(\epsilon, L, \alpha, \phi_0, T), \tag{9}$$

where $\omega_{\alpha,0}(\theta) = (1-\theta)\omega_\alpha(\theta)$*,* ω_α *is given in* (4) *and*

$$C(\epsilon, L, \alpha, \phi_0, T) = 2\left(\phi_0^2\alpha e^{2\epsilon T} + \left(\frac{L^2}{4\epsilon}\alpha + (L^2+\phi_0^2)(1-\alpha)\right)\frac{e^{2\epsilon T}-1}{\epsilon}\right).$$

Temporal-discretization scheme

- In the section, we mainly consider the case $F(t, \phi(t)) = \lambda \mathcal{C}[\varphi](t)$.
- Multiplying $1-\theta$ on both sides of EIDEs (8), we get the BDF-k scheme for (8) as follows:

$$\frac{1-\theta}{\Delta t}\left(\alpha_k \varphi^{n+1}(\theta) - \sum_{j=0}^{k-1} b_j^{(k)} \varphi^{n-j}(\theta)\right) + \theta\varphi^{n+1}(\theta) = \lambda \mathcal{C}[\varphi^{n+1}] + \theta\phi_0, \tag{10}$$

where α_k and $b_j^{(k)}$ $(k = 1, 2, 3, 4, 5)$ are given in Table 1.

k	α_k	$b_0^{(k)}$	$b_1^{(k)}$	$b_2^{(k)}$	$b_3^{(k)}$	$b_4^{(k)}$
1	1	1				
2	$\frac{3}{2}$	2	-$\frac{1}{2}$			
3	$\frac{11}{6}$	3	-$\frac{3}{2}$	$\frac{1}{3}$		
4	$\frac{25}{12}$	4	-3	$\frac{4}{3}$	-$\frac{1}{4}$	
5	$\frac{137}{60}$	5	-5	$\frac{10}{3}$	-$\frac{5}{4}$	$\frac{1}{5}$

Table: The BDF-k coefficients α_k and $b_j^{(k)}$

Stability

Theorem

The semi-discrete BDF-k $(1 \leq k \leq 5)$ scheme (10) *is stable with $\lambda \leq 0$ in the sense that,*

$$\lambda_{min}\|\varphi^{N+1}\|^2_{L^2_{\omega_{\alpha,0}}} + \frac{\Delta t}{2}(1-\tau_k^2)\sum_{n=k-1}^{N}\|\varphi^{n+1}\|^2_{L^2_{\omega_{\alpha,1}}} + \frac{\Delta t|\lambda|}{2}(1-\tau_k^2)\sum_{n=k-1}^{N}|\phi^{n+1}|^2 \leq \frac{1}{1-\tau_k^2}\left[2\lambda_{max}\alpha + T(1-\alpha)\right]|\phi_0|^2, \tag{11}$$

where$0 \leq \tau_k < 1$, ϕ_0 is the initial value, λ_{min} and λ_{max} are the minimum eigenvalue and the maximum eigenvalue of the positive definite symmetric matrix $G = (g_{ij})$, respectively.

Spectral collocation method

- Let $\{\theta_j\}_{j=0}^{M}$ be the Jacobi-Gauss points in $[0,1]$ with respect to the weight $\Gamma(\alpha)\Gamma(1-\alpha)\omega_\alpha(\theta) = \theta^{-\alpha}(1-\theta)^{\alpha-1}$, and $\{h_j(\theta)\}_{j=0,M}$ be the Lagrange interpolation functions with respect to the Jacobi-Gauss points $\{\theta_j\}_{j=0}^{M}$, respectively. We then approximate the function $\varphi^n(\theta)$ by

$$\varphi_M^n(\theta) = \sum_{j=0}^{M} \varphi^n(\theta_j) h_j(\theta),$$

and compute the function $\phi_M^n := \mathcal{C}[\varphi_M^n]$ by using the Gauss-Jacobi quadrature, namely,

$$\mathcal{C}[\varphi_M^n] = \int_0^1 \varphi_M^n(\theta)\omega_\alpha(\theta)d\theta = \sum_{j=0}^{M} \varphi_M^n(\theta_j)\omega_j, \tag{12}$$

where $\omega_j = \int_0^1 h_j(\theta)\omega_\alpha(\theta)d\theta$, $j = 0, \cdots, M$ are the corresponding Jacobi-Guass weights.

Spectral collocation method

- Now we have the spectral collocation scheme for the semi-discrete problem (10): for $0 \le s \le M$,

$$\frac{(1-\theta_s)}{\Delta t}\left(\alpha_k \varphi_M^{n+1}(\theta_s) - \sum_{j=0}^{k-1} b_j^{(k)} \varphi_M^{n-j}(\theta_s)\right) + \theta_s \varphi_M^{n+1}(\theta_s) \tag{13}$$
$$= \lambda \mathcal{C}[\varphi_M^{n+1}] + \theta_s \phi_0.$$

- Denote P_M the set of all algebraic polynomials of degree $\le M$, we have $P_M = \text{span}\{h_j(\theta) : 0 \le j \le M\}$. Then the spectral collocation formula is equivalent to the following Galerkin form: Find $\varphi_M^{n+1} \in P_M$, such that

$$\left(\alpha_k \varphi_M^{n+1} - \sum_{j=0}^{k-1} b_j^{(k)} \varphi_M^{n-k}, q_M\right)_{L^2_{\omega_{\alpha,0}}} + \Delta t(\varphi_M^{n+1}, q_M)_{L^2_{\omega_{\alpha,1}}} \tag{14}$$
$$= \Delta t \lambda \left(\mathcal{C}[\varphi_M^{n+1}], q_M\right)_{L^2_{\omega_\alpha}} + \Delta t(\phi_0, q_M)_{L^2_{\omega_{\alpha,1}}} \quad \forall q_M \in P_M.$$

Stability

Therefore, by using the same argument as that used for Theorem 2, we conclude that the fully discretization scheme (13) is also stable.

Theorem

The fully-discrete BDF-k $(1 \leq k \leq 5)$ *scheme* (13) *is stable with* $\lambda \leq 0$ *in the sense that,*

$$
\begin{aligned}
&\lambda_{min}\|\varphi_M^{N+1}\|^2_{L^2_{\omega_{\alpha,0}}} + \frac{\Delta t}{2}(1-\tau_k^2)\sum_{n=k-1}^{N}\|\varphi_M^{n+1}\|^2_{L^2_{\omega_{\alpha,1}}} \\
&+\frac{\Delta t|\lambda|}{2}(1-\tau_k^2)\sum_{n=k-1}^{N}\left|\mathcal{C}[\varphi_M^{n+1}]\right|^2 \\
&\leq \frac{1}{1-\tau_k^2}\Big[2\lambda_{max}\alpha + T(1-\alpha)\Big]|\phi_0|^2.
\end{aligned}
\tag{15}
$$

Implementation

- Now let us briefly give a description for the efficient implementation. We write the scheme (13) into the following matrix form

$$\mathbf{A}\boldsymbol{\Phi}^{n+1} = \sum_{j=0}^{k-1} \mathbf{B}_j \boldsymbol{\Phi}^{n-j} + \mathbf{F}, \tag{16}$$

where

$$\begin{aligned}
&\mathbf{A} = \mathrm{diag}(A) - \Delta t \lambda \mathbf{J}_{M+1}\mathbf{W}, \quad \mathbf{B}_j = b_j^{(k)}\mathrm{diag}(B) \\
&A = [\alpha_k(1-\theta_0) + \Delta t\theta_0, \cdots, \alpha_k(1-\theta_M) + \Delta t\theta_M]^T, \\
&B = [1-\theta_0, \cdots, 1-\theta_M]^T, \quad \mathbf{F} = \Delta t\phi_0 [\theta_0, \cdots, \theta_M]^T, \\
&\mathbf{W} = \mathrm{diag}(W), \quad W = [\omega_0, \cdots, \omega_{M+1}]^T, \\
&\boldsymbol{\Phi}^j = \left[\varphi^j(\theta_0), \cdots, \varphi^j(\theta_{M+1})\right]^T,
\end{aligned}$$

and Δt is time step, $\mathbf{J}_{M+1}$ is the all-one $(M+1)\times(M+1)$ matrix.

- Due to the stability of the scheme (13), we have that $\mathbf{A}$ is non-singular. Then we have the following characteristic decomposition of $\mathbf{A}$:

$$\mathbf{X}\boldsymbol{\Lambda}\mathbf{X}^{-1} = \mathbf{A}, \tag{17}$$

where $\mathbf{X}$ is the matrix whose columns are the corresponding eigenvectors of $\mathbf{A}$ and $\boldsymbol{\Lambda}$ is the diagonal matrix whose diagonal entries are the eigenvalues of $\mathbf{A}$, respectively. Multiply both sides of (16) with $\mathbf{X}^{-1}$ and define the vectors

$$\mathbf{Y} = \mathbf{X}^{-1}\boldsymbol{\Phi}^{n+1}, \quad \hat{\mathbf{Y}} = \boldsymbol{\Lambda}\mathbf{Y}, \tag{18}$$

we have

$$\hat{\mathbf{Y}} = \boldsymbol{\Lambda}\mathbf{Y} = \mathbf{X}^{-1}\left(\sum_{j=0}^{k-1}\mathbf{B}_j\boldsymbol{\Phi}^{n-j} + \mathbf{F}\right), \tag{19}$$

- We summarize the implementation in the following algorithm:

Algorithm 3.1 Efficient implementation for the fully-discrete scheme (3.10)

Input: $\mathbf{A}$, $\mathbf{B}_j$, $\mathbf{\Phi}^{n-j}$, $j = 0, \ldots, k-1$
Output: $\mathbf{\Phi}^{n+1}$
1: We compute $\mathbf{X}^{-1}$ and $\mathbf{\Lambda}$ by $\mathbf{X\Lambda X}^{-1} = \mathbf{A}$
2: **for** $n = k-1, \cdots, N$ **do**
3: We compute $\hat{\mathbf{Y}}$ by $\hat{\mathbf{Y}} = \mathbf{X}^{-1}\left(\sum_{j=0}^{k-1} \mathbf{B}_j \mathbf{\Phi}^{n-j} + \mathbf{F}\right)$
4: We compute $\mathbf{Y}$ by $\hat{\mathbf{Y}} = \mathbf{\Lambda Y}$
5: We compute $\mathbf{\Phi}^{n+1}$ by $\mathbf{\Phi}^{n+1} = \mathbf{XY}$
6: **end for**
7: **return** $\mathbf{\Phi}^{n+1}$

Error estimate of the spectral collocation method

Theorem

Assume $\varphi(t,\theta) \in L^2(I; B^m_{\alpha-1,-\alpha}(\Omega))$, $0 \le m \le M$, *then we have for* $n \ge 0$ *that*

$$\begin{aligned} & \|\varphi(t_{n+1},\theta) - \varphi_M(t_{n+1},\theta)\|^2_{L^2_{\omega_\alpha}} + |\lambda||\mathcal{C}[\varphi - \varphi_M](t_{n+1})|^2 \\ & \le CM^{-2m}\Big(\int_0^{t_{n+1}} \|\frac{\partial^m \varphi(\tau,\theta)}{\partial \theta^m}\|^2_{\omega^{\alpha-1+m,-\alpha+m}} d\tau \\ & + \int_0^{t_{n+1}} \|\frac{\partial^{m+1}\varphi(t,\theta)}{\partial\theta^m \partial t}\|^2_{\omega^{\alpha-1+m,-\alpha+m}} d\tau \Big). \end{aligned} \tag{20}$$

Error estimate for the time discretization

Theorem

Assume $\frac{\partial^{k+1}\varphi_M(t,\theta)}{\partial t^{k+1}} \in L^2(I; L^2_{\omega_{\alpha,0}}(\Omega))$, $1 \le k \le 5$, *then we have*

$$\begin{aligned}
&\lambda_{min}\|\varphi_M(t_{N+1},\theta) - \varphi_M^{N+1}\|^2_{L^2_{\omega_{\alpha,0}}} \\
&+\frac{\Delta t}{2}(1-\tau_k^2)\sum_{n=k-1}^{N}\|\varphi_M(t_{n+1},\theta) - \varphi_M^{n+1}\|^2_{L^2_{\omega_{\alpha,1}}} \\
&+\frac{\Delta t|\lambda|}{2}(1-\tau_k^2)\sum_{n=k-1}^{N}\left|\mathcal{C}[\varphi_M](t_{n+1}) - \mathcal{C}[\varphi_M^{n+1}]\right|^2 \\
&\le \frac{CT}{4\xi^2}\Delta t^{2k}\int_0^{t_{N+1}}\|\frac{\partial^{k+1}\varphi_M(\tau,\theta)}{\partial \tau^{k+1}}\|^2_{L^2_{\omega_{\alpha,0}}}d\tau.
\end{aligned} \tag{21}$$

Error estimate

By the triangle inequality and Theorem 4 and Theorem 5 to obtain the following error estimate:

Theorem

Assume $\varphi \in L^2(I; B^m_{\alpha-1,-\alpha}(\Omega))$, $\frac{\partial^{k+1}\varphi_M}{\partial^{k+1}t} \in L^2(I; L^2_{\omega_{\alpha,0}}(\Omega))$,$0 \le m \le M$, $1 \le k \le 5$, *then we have*

$$
\begin{aligned}
&\Delta t \sum_{n=k-1}^{N} \|\varphi(t_{n+1},\theta) - \varphi_M^{n+1}\|^2_{L^2_{\omega_\alpha}} \\
&\le CM^{-2m} \int_0^{t_{N+1}} \Big(\| \frac{\partial^m \varphi(t,\theta)}{\partial \theta^m} \|^2_{\omega^{\alpha-1+m,-\alpha+m}} \\
&+ \| \frac{\partial^{m+1}\varphi(\tau,\theta)}{\partial\theta^m \partial t} \|^2_{\omega^{\alpha-1+m,-\alpha+m}} \Big) d\tau \\
&+ \frac{CT}{4\xi^2} \Delta t^{2k} \int_0^{t_{N+1}} \| \frac{\partial^{k+1}\varphi_M(\tau,\theta)}{\partial \tau^{k+1}} \|^2_{L^2_{\omega_{\alpha,0}}} d\tau.
\end{aligned}
$$

Linear case

- Example 1:Consider the linear problem

$$\frac{d^\alpha \phi}{dt^\alpha} = F(t, \phi(t)), \quad t > 0, \quad \phi(0) = \phi_0,$$

where

$$F(t, \phi(t)) = \lambda \phi(t) + f(t).$$

The following three cases are consider:

- Case I:$f(t) = \Gamma(1+\alpha)$, $\lambda = 0$, and the exact solution is taken as $\phi(t) = t^\alpha$.
- Case II:$f(t) = 0$, $\lambda = -1$, and the exact solution is $\phi(t) = E_\alpha(\lambda t^\alpha)$, where $E_\alpha(t)$ is the Mittag-Leffler function.
- Case III:$f(t) = sin(t)$, $\lambda = -1$, and the initial value is $\phi_0 = 1$.

Example 1: Convergence results for θ

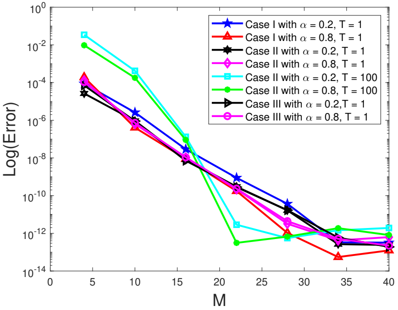
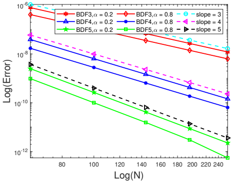
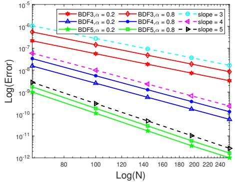


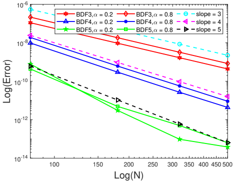
Figure: Example 1. Convergence results for the spectral approximation of the extended θ direction for $\alpha = 0.2$, 0.8 and different times T. Here we set Δt to be small enough. We obtain spectral accuracy for all test cases.



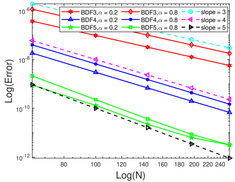
(a) Case I: $T = 1$



(b) Case II: $T = 1$



(c) Case II: $T = 20$



(d) Case III: $T = 1$

Figure: Example 1. Convergence results for the BDF-k ($k = 3, 4, 5$) time discretization schemes for different values of fractional order $\alpha = 0.2$, 0.8 and different times T. Here we set $M = 30$. The results are consistent with Theorem

Nonlinear case

- Example 2:Consider the nonlinear problem

$$F(t, \phi(t)) = \lambda\phi^3(t) + f(t).$$

The following two cases are consider:

- Case IV: $f(t) = \frac{\Gamma(3+\alpha)}{2}t^2 - \lambda t^{6+3\alpha}$, $\lambda \neq 0$, and the exact solution is $\phi(t) = t^{2+\alpha}$.
- Case V:$f(t) = 0$,$\lambda = -1$,and the initial value is $\phi_0 = 1$.

Example 2: Convergence results for θ

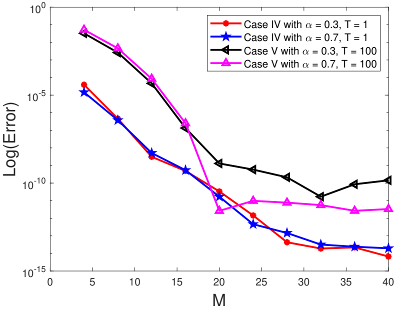
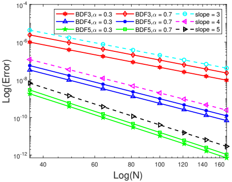
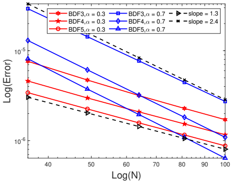


Figure: Example 2. Convergence results for the spectral approximation of the extended θ direction for $\alpha = 0.3$, 0.7 and different times T. Here we set Δt to be small enough. We obtain spectral accuracy for all test cases.

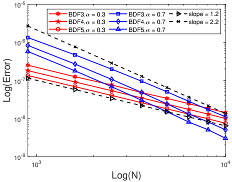
Example 2: Convergence results for temporal



(a) Case IV: $T = 1$



(b) Case V: $T = 1$



(c) Case V: $T = 100$

Figure: Example 2. Convergence results for the BDF-k ($k = 3, 4, 5$) time discretization schemes for different values of fractional order $\alpha = 0.3$, 0.7 and different times T. Here we set $M = 30$.

Conclusion

- We show the equivalence between FDEs and the *Extended Integer Differential Equation*(EIDE), and establish the stability of EIDE.
- We apply BDF-k formula for the temporal discretization while we use the Jacobi spectral collocation method for the discretization of the extended direction. We analyze the stability of the proposed method and give rigorous error estimates with order $O(\Delta t^k + M^{-m})$, where Δt and M are time step size and number of collocation nodes in extended direction, respectively. We point out that the computational cost and storage requirement of our numerical schemes are $O(1)$.
- We demonstrated the effectiveness of our method by linear and non-linear examples.

Thank you for your attention!