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HIGH-ORDER BDF CONVOLUTION QUADRATURE FOR SUBDIFFUSION MODELS WITH A SINGULAR SOURCE TERM*

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Abstract. Anomalous diffusion is often modelled in terms of the subdiffusion equation, which can involve a weakly singular source term. For this case, many predominant time-stepping methods, including the correction of high-order backward differentiation formula (BDF) schemes [B. Jin, B. Y. Li, and Z. Zhou, *SIAM J. Sci. Comput.,* 39 (2017), pp. A3129–A3152], may suffer from a severe order reduction. To fill in this gap, we propose a smoothing method for time-stepping schemes, where the singular term is regularized by using an m-fold integral-differential calculus and the equation is discretized by the k-step BDF convolution quadrature, called the IDm-BDFk method. We prove that the desired kth-order convergence can be recovered even if the source term is weakly singular and the initial data is not compatible. Numerical experiments illustrate the theoretical results.

Key words. subdiffusion equation, smoothing method, IDm-BDFk method, singular source term, error estimate

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1. Introduction.

In this paper we study the convolution quadrature generated by the k-step backward differentiation formulas (BDFk) for solving the subdiffusion model with a weakly singular source term, whose prototype equation is, for $0 < \alpha < 1$,

$$\partial_t^\alpha (u(t) - v) - Au(t) = g(t) := t^\mu \circ f(t), \ \mu > -1 \tag{1.1}$$

with the initial condition $u(0) = v$. The operator A denotes the Laplacian Δ on a convex polyhedral domain $\Omega \subset \mathbb{R}^d$ with a homogenous Dirichlet boundary condition, and $\mathcal{D}(A) = H_0^1(\Omega) \cap H^2(\Omega)$, where $H_0^1(\Omega)$, $H^2(\Omega)$ denote the standard Sobolev spaces. The symbol $\circ$ can be either the convolution $*$ or the product, and the Riemann–Liouville fractional derivative is defined by [21, p. 62]

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t (t-\tau)^{-\alpha} u(\tau) d\tau.$$

It makes sense to allow $\partial_t^\alpha u(t)$ to be singular at $t = 0$ if u is absolutely continuous. This leads to the fractional differential equations involving a singular source term; see [22, eq. (20)], [7, eq. (7.24)], [10, eq. (4.22)], and [17, eq. (1.6)].

Problems of the model (1.1) arise in a variety of physical, chemical, and geophysical applications [8, 16, 18, 22, 23]. As an example, a singular fractal mobile/immobile model for solute transport [22] has important applications in practice, and has been applied successfully to geophysical systems such as groundwater aquifers, rivers, and porous media [8, 23].

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Numerical methods for the time discretization of (1.1) have been investigated by various authors. Nowadays, there exist two predominant time-stepping schemes to restore the high-order convergence rate for the model (1.1). The first type is that the nonuniform meshes (e.g., graded meshes, geometric meshes) are employed to capture the weak singularities at $t=0$ under the appropriate regularity of the solution; see [2, 13, 14, 19, 20, 27]. The second type is convolution quadrature. For example, an usual approach for the source term $g(t)$ in (1.1) is to write

$$g(t)=g(0)+\sum_{l=1}^{k-1}\frac{t^l}{l!}\partial_t^l g(0)+\frac{t^{k-1}}{(k-1)!}*\partial_t^k g(t).$$

Then approximating $g(0)=\partial_t J^1 g(0)$ by $\partial_\tau J^1 g(0)$ may yield a modified BDF2 method with correction in the first step [6]. Furthermore, the correction of high-order BDFk or L_k methods is well developed in [12, 25, 26, 32] under the mild regularity of the source function g. For the low regularity source term $g(t)=t^\mu$, $\mu>0$, the correction of high-order BDFk schemes converges with the order $\mathcal{O}(\tau^{1+\mu})$ (see Lemma 3.2 in [31]), which may lose the high-order accuracy and exhibit a severe order reduction. For the weakly singular source function $g(t)=t^\mu$, $\mu>-1$, a second-order time-stepping method is provided in [33] by performing the integral-differential calculus on both sides of (1.1). For the general function $g(t)=t^\mu f(t)$, $\mu>-1$, the second-order schemes are well developed in [4] just by performing the integral-differential operator for the source term g. However, it may not offer an important insight into the causes of high-order BDF convolution quadrature for the subdiffusion model (1.1). For example, an optimal error estimate of the Newton–Cotes [3, 28] rule $\mathcal{O}\left(\tau^{\min\{m+1,k\}}\right)$ for odd m and $\mathcal{O}\left(\tau^{\min\{m+2,k\}}\right)$ for even m, $1\le m\le k\le 6$, is difficult to illustrate; see Theorem 3.8.

How to design/restore the desired kth-order convergence rate of the k-step BDF ($k\le 6$) convolution quadrature with a weakly singular source term for the model (1.1) still has not been addressed in the literature. To fill in this gap, we propose and analyze a smoothing method for the time-stepping schemes, where the singular term is regularized by using an m-fold integral-differential calculus and the equation is discretized by the k-step BDF convolution quadrature, called the IDm-BDFk method or smoothing method. We prove that the desired kth-order convergence can be recovered even if the source term is weakly singular and the initial data is not compatible. Numerical experiments illustrate the theoretical results.

2. IDm-BDFk method (smoothing method).

Let $V(t)=u(t)-v$ with $V(0)=0$. Then we can rewrite (1.1) as

$$\partial_t^\alpha V(t)-AV(t)=Av+g(t),\quad 0<t\le T. \tag{2.1}$$

It is well known that the operator A satisfies the resolvent estimate [15, 29]

$$\left\|(z-A)^{-1}\right\|\le c|z|^{-1}\quad \forall z\in\Sigma_\theta,$$

for all $\theta\in(\pi/2,\pi)$. Here $\Sigma_\theta:=\{z\in\mathbb{C}\backslash\{0\}:|\arg z|<\theta\}$ is a sector of the complex plane $\mathbb{C}$. It means that $z^\alpha\in\Sigma_{\theta'}$, $\theta'=\alpha\theta<\theta<\pi$ for all $z\in\Sigma_\theta$, and

$$\left\|\left(z^\alpha-A\right)^{-1}\right\|\le c|z|^{-\alpha}\quad \forall z\in\Sigma_\theta. \tag{2.2}$$

Here and below $\|\cdot\|$ and $\|\cdot\|_{L^2(\Omega)}$ denote the operator norm [29, p. 91] and usual norm [29, p. 2] in the space $L^2(\Omega)$, respectively.

2.1. Discretization schemes. Let the m-fold integral calculus [21, p. 64]

$$G(t) = J^m g(t) = \frac{1}{\Gamma(m)} \int_0^t (t-\tau)^{m-1} g(\tau) d\tau = \frac{t^{m-1}}{\Gamma(m)} * g(t), \ 1 \le m \le k \le 6. \tag{2.3}$$

Note that $G(t)$ is a smooth function and satisfies $G(0) = J^m g(t)|_{t=0} = 0$. Here J may map a singular point of g to a zero point of G. The model (2.1) then becomes

$$\partial_t^\alpha V(t) - AV(t) = \partial_t^m \left(\frac{t^m}{m!} Av + G(t) \right), \quad 0 < t \le T. \tag{2.4}$$

Let $N \in \mathbb{N}$, $\tau = \frac{T}{N}$ be the uniform time step, and $t_n = n\tau$, $n = 0, 1, \ldots, N$, be a uniform partition of the interval $[0, T]$. Denote u^n as the approximated value of $u(t)$ at $t = t_n$ and $g^n = g(t_n)$. The convolution quadrature generated by BDFk approximates the Riemann–Liouville fractional derivative $\partial_t^\alpha \varphi(t_n)$ by

$$\partial_{\tau,k}^\alpha \varphi^n = \frac{1}{\tau^\alpha} \sum_{j=0}^n \omega_j^{(\alpha,k)} \varphi^{n-j}, \ 1 \le k \le 6. \tag{2.5}$$

Here the weights $\omega_j^{(\alpha,k)}$ are the coefficients in the series expansion

$$\delta_{\tau,k}^\alpha(\xi) = \frac{1}{\tau^\alpha} \sum_{j=0}^\infty \omega_j^{(\alpha,k)} \xi^j \quad \text{with} \quad \delta_{\tau,k}(\xi) = \frac{1}{\tau} \sum_{j=1}^k \frac{1}{j} (1-\xi)^j, \tag{2.6}$$

which can be computed by the fast Fourier transform [21, Chapter 7] or recursion [5].

Then the IDm-BDFk method for (2.4) is designed by

$$\partial_{\tau,k}^\alpha V^n - AV^n = \partial_{\tau,k}^m \left(\frac{t_n^m}{m!} Av + G^n \right), \ 1 \le m \le k \le 6. \tag{2.7}$$

Remark 2.1. For the time semidiscrete schemes (2.7), we require $v \in \mathcal{D}(A)$. However, one can use the schemes (2.7) to prove the error estimates with the nonsmooth data $v \in L^2(\Omega)$; see Theorem 5.5. In this work, we mainly focus on the time semidiscrete schemes (2.7), since the spatial discretization is well understood. In fact, we can choose $v_h = R_h v$ if $v \in \mathcal{D}(A)$ and $v_h = P_h v$ if $v \in L^2(\Omega)$; see [26, 29, 30].

2.2. Continuous solution representation for (2.4). Applying the Laplace transform in (2.4) yields

$$\widehat{V}(z) = (z^\alpha - A)^{-1} \left(z^{-1} Av + z^m \widehat{G}(z) \right).$$

By the inverse Laplace transform, we obtain [12]

$$V(t) = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}} e^{zt} (z^\alpha - A)^{-1} \left(z^{-1} Av + z^m \widehat{G}(z) \right) dz \tag{2.8}$$

with

$$\Gamma_{\theta,\kappa} = \{ z \in \mathbb{C} : |z| = \kappa, |\arg z| \le \theta \} \cup \{ z \in \mathbb{C} : z = re^{\pm i\theta}, r \ge \kappa \} \tag{2.9}$$

and $\theta \in (\pi/2, \pi)$, $\kappa > 0$.

2.3. Discrete solution representation for (2.7). Given a sequence $(\kappa^n)_0^\infty$ we denote by

$$\widetilde{\kappa}(\zeta) = \sum_{n=0}^{\infty} \kappa^n \zeta^n$$

its generating power series. Then we have the following result.

LEMMA 2.1. *Let $\delta_{\tau,k}$ be given in (2.6) and $G(t) = J^m g(t)$, $1 \le m \le k \le 6$ in (2.3). Then the discrete solution of (2.7) is represented by*

$$V^n = \frac{\tau}{2\pi i} \int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n} \left(\delta^\alpha_{\tau,k}(e^{-z\tau}) - A\right)^{-1} \delta^m_{\tau,k}(e^{-z\tau}) \left(\frac{\gamma_m(e^{-z\tau})}{m!} \tau^m A v + \widetilde{G}(e^{-z\tau}) \right) dz$$

with $\Gamma^\tau_{\theta,\kappa} = \{z \in \Gamma_{\theta,\kappa} : |\Im z| \le \pi/\tau\}$ and $\gamma_m(\xi) = \sum_{n=1}^\infty n^m \xi^n = \left(\xi \frac{d}{d\xi}\right)^m \frac{1}{1-\xi}$.

Proof. Multiplying (2.7) by ξ^n and summing over n, we obtain

$$\sum_{n=1}^{\infty} \partial^\alpha_{\tau,k} V^n \xi^n - \sum_{n=1}^{\infty} A V^n \xi^n = \sum_{n=1}^{\infty} \partial^m_{\tau,k} \left(\frac{t_n^m}{m!} A v + G^n \right) \xi^n.$$

From (2.5), (2.6), and $V^0 = 0$, there exists

$$\sum_{n=1}^{\infty} \partial^\alpha_{\tau,k} V^n \xi^n = \sum_{n=1}^{\infty} \frac{1}{\tau^\alpha} \sum_{j=0}^{n} \omega_j^{(\alpha,k)} V^{n-j} \xi^n = \frac{1}{\tau^\alpha} \sum_{j=0}^{\infty} \omega_j^{(\alpha,k)} \xi^j \sum_{n=0}^{\infty} V^n \xi^n = \delta^\alpha_{\tau,k}(\xi) \widetilde{V}(\xi).$$

Similarly, by the identities $\gamma_m(\xi) = \sum_{n=1}^\infty n^m \xi^n$, $m \ge 1$, and $G^0 = G(0) = 0$, we get

$$\sum_{n=1}^{\infty} \partial^m_{\tau,k} t_n^m A v \xi^n = \delta^m_{\tau,k}(\xi) \gamma_m(\xi) \tau^m A v, \quad \sum_{n=1}^{\infty} \partial^m_{\tau,k} G^n \xi^n = \delta^m_{\tau,k}(\xi) \widetilde{G}(\xi).$$

According to the above equations, this yields

$$\widetilde{V}(\xi) = \left(\delta^\alpha_{\tau,k}(\xi) - A\right)^{-1} \delta^m_{\tau,k}(\xi) \left(\frac{\gamma_m(\xi)}{m!} \tau^m A v + \widetilde{G}(\xi) \right). \tag{2.10}$$

From Cauchy's integral formula, the change of variables $\xi = e^{-z\tau}$, and Cauchy's theorem, this implies [12]

$$V^n = \frac{\tau}{2\pi i} \int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n} \left(\delta^\alpha_{\tau,k}(e^{-z\tau}) - A\right)^{-1} \delta^m_{\tau,k}(e^{-z\tau}) \left[\frac{\gamma_m(e^{-z\tau})}{m!} \tau^m A v + \widetilde{G}(e^{-z\tau}) \right] dz \tag{2.11}$$

with $\Gamma^\tau_{\theta,\kappa} = \{z \in \Gamma_{\theta,\kappa} : |\Im z| \le \pi/\tau\}$. The proof is completed. ∎

3. Convergence analysis: General source function $g(t)$. Based on the framework of convolution quadrature [4, 12, 25], we first provide the detailed error analysis for the subdiffusion model (2.1) with the general source function $g(t)$.

3.1. A few technical lemmas. We give some lemmas that will be used. First, we need a few estimates on $\delta_{\tau,k}(e^{-z\tau})$ in (2.6).

LEMMA 3.1 (see [12]). *Let $\delta_{\tau,k}(\xi)$ with $k\le 6$ be given in* (2.6). *Then there exist the positive constants c_1, c_2, c, ε, and $\theta\in(\pi/2,\theta_\varepsilon)$ with $\theta_\varepsilon\in(\pi/2,\pi)$ such that*

$$c_1|z|\le|\delta_{\tau,k}(e^{-z\tau})|\le c_2|z|,\quad |\delta_{\tau,k}(e^{-z\tau})-z|\le c\tau^k|z|^{k+1},$$
$$|\delta^\alpha_{\tau,k}(e^{-z\tau})-z^\alpha|\le c\tau^k|z|^{k+\alpha},\ \delta_{\tau,k}(e^{-z\tau})\in\Sigma_{\pi/2+\varepsilon}\quad \forall z\in\Gamma^\tau_{\theta,\kappa},$$

where $\theta\in(\pi/2,\pi)$ is sufficiently close to $\pi/2$.

To provide an optimal error estimate of the Newton–Cotes rule for the IDm-BDFk, the following lemmas will play an important role.

LEMMA 3.2. *Let $\gamma_l(\xi)=\sum_{n=1}^\infty n^l\xi^n$ with $l=0,1,2,\dots,2k$, $k\le 6$. Then there exists a positive constant c such that*

$$\left|\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-\frac{1}{z^{l+1}}\right|\le\begin{cases} c\tau^{l+1}, & l=0 \text{ or } l=1,3,\dots,2k-1,\\ c\tau^{l+2}|z|, & l=2,4,\dots,2k.\end{cases}$$

Proof. Taking $\xi=e^{-z\tau}$, we get

$$\gamma_l(\xi)=\sum_{n=1}^\infty n^l\xi^n=\frac{\sum_{j=0}^l a_{l,j}\xi^{l+1-j}}{(1-\xi)^{l+1}},\ l\ge 0,$$

with $a_{0,0}=1$, $a_{0,1}=0$, and

$$a_{l,j}=ja_{l-1,j}+(l+1-j)a_{l-1,j-1},\ a_{l,0}=a_{l,l+1}=0,\ l\ge 1.$$

In particular, we have $a_{l,j}=a_{l,l+1-j}$, $l\ge 1$, and

$$\gamma_l(\xi)=\frac{\sum_{j=1}^l a_{l,l+1-j}\xi^{l+1-j}}{(1-\xi)^{l+1}}=\frac{\sum_{j=1}^l a_{l,j}\xi^j}{(1-\xi)^{l+1}}.$$

By the simple calculation, this yields

$$\left|\frac{\gamma_l(e^{-\eta})}{l!}\eta^{l+1}-1\right|\le\begin{cases} c|\eta|^{l+1}, & l=0 \text{ or } l=1,3,\dots,2k-1,\\ c|\eta|^{l+2}, & l=2,4,\dots,2k,\end{cases}$$

since

$$\frac{\gamma_l(e^{-\eta})}{l!}\eta^{l+1}=\frac{e^{-\eta}}{(1-e^{-\eta})\,\eta^{-1}}=\frac{1-\frac{\eta}{1!}+\frac{\eta^2}{2!}-\frac{\eta^3}{3!}+\cdots}{1-\frac{\eta}{2!}+\frac{\eta^2}{3!}-\frac{\eta^3}{4!}+\cdots},\quad l=0,$$

and

$$\frac{\gamma_l(e^{-\eta})}{l!}\eta^{l+1}=\frac{\frac{1}{l!}\sum_{j=1}^l a_{l,j}e^{\left(\frac{l+1}{2}-j\right)\eta}}{\left(e^{\frac{\eta}{2}}-e^{-\frac{\eta}{2}}\right)^{l+1}\eta^{-(l+1)}}=\frac{1+c_2\eta^2+c_4\eta^4+c_6\eta^6+\cdots}{1+d_2\eta^2+d_4\eta^4+d_6\eta^6+\cdots}\quad\forall l\ge 1$$

with $c_{2i}=d_{2i}$, $2i\le l$. Here the coefficients c_{2i} and d_{2i}, $i=1,2,\dots$, are computed by

$$c_{2i}=\frac{1}{l!}\sum_{j=1}^l a_{l,j}\frac{1}{(2i)!}\left(\frac{l+1}{2}-j\right)^{2i}$$

and

$$d_{2i}=\frac{1}{(2i+l+1)!}\sum_{j=0}^{l+1}(-1)^j\binom{l+1}{j}\left(\frac{l+1}{2}-j\right)^{2i+l+1}.$$

The proof is completed. ∎

LEMMA 3.3. *Let $\delta_{\tau,k}(\xi)$ be given in* (2.6) *and $\gamma_l(\xi)=\sum_{n=1}^{\infty} n^l\xi^n$ with $l=0,1,\ldots,k+m$, $1\le m\le k\le 6$. Then there exists a positive constant c such that*

$$\left|\delta_{\tau,k}^m(e^{-z\tau})\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-\frac{z^m}{z^{l+1}}\right|\le\begin{cases} c\tau^{l+1}\left|z\right|^m+c\tau^k|z|^{k+m-l-1}, & l=0,1,3,\ldots,\\ c\tau^{l+2}\left|z\right|^{m+1}+c\tau^k|z|^{k+m-l-1}, & l=2,4,\ldots. \end{cases}$$

Proof. Let

$$\delta_{\tau,k}^m(e^{-z\tau})\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-\frac{z^m}{z^{l+1}}=J_1+J_2$$

with

$$J_1=\delta_{\tau,k}^m\left(e^{-z\tau}\right)\left(\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-\frac{1}{z^{l+1}}\right)\quad\text{and}\quad J_2=\frac{\delta_{\tau,k}^m(e^{-z\tau})-z^m}{z^{l+1}}.$$

From Lemmas 3.1 and 3.2, this leads to

$$|J_1|\le\begin{cases} c\tau^{l+1}\left|z\right|^m, & l=0\text{ or }l=1,3,\ldots,2k-1,\\ c\tau^{l+2}\left|z\right|^{m+1}, & l=2,4,\ldots,2k, \end{cases}$$

and

$$|J_2|\le c\tau^k|z|^{k+1}|z|^{m-1}|z|^{-l-1}\le c\tau^k|z|^{k+m-l-1}.$$

By the triangle inequality, the desired result is obtained. ◻

From Lemmas 3.1–3.3, we have the following results, which will be used in the global convergence analysis.

LEMMA 3.4. *Let $\delta_{\tau,k}^\alpha$ be given in* (2.6) *and $\gamma_l(\xi)=\sum_{n=1}^{\infty} n^l\xi^n$, $l=0,1,\ldots,k+m$, $1\le m\le k\le 6$. Then there exists a positive constant c such that*

$$\|K(z)\|\le\begin{cases} c\tau^{l+1}\left|z\right|^{m-\alpha}+c\tau^k|z|^{k+m-l-1-\alpha}, & l=0\text{ or }l=1,3,\ldots,2k-1,\\ c\tau^{l+2}\left|z\right|^{m+1-\alpha}+c\tau^k|z|^{k+m-l-1-\alpha}, & l=2,4,\ldots,2k, \end{cases}$$

with

$$K(z)=\left(\delta_{\tau,k}^\alpha(e^{-z\tau})-A\right)^{-1}\delta_{\tau,k}^m(e^{-z\tau})\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-(z^\alpha-A)^{-1}\frac{z^m}{z^{l+1}}.$$

Proof. Let $K(z)=I+II$ with

$$\begin{aligned} I&=\left(\delta_{\tau,k}^\alpha(e^{-z\tau})-A\right)^{-1}\left[\delta_{\tau,k}^m(e^{-z\tau})\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-\frac{z^m}{z^{l+1}}\right],\\ II&=\left[\left(\delta_{\tau,k}^\alpha(e^{-z\tau})-A\right)^{-1}-(z^\alpha-A)^{-1}\right]\frac{z^m}{z^{l+1}}. \end{aligned}$$

The resolvent estimate (2.2) and Lemmas 3.1 and 3.3 imply directly

$$\|\left(\delta_{\tau,k}^\alpha(e^{-z\tau})-A\right)^{-1}\|\le c|z|^{-\alpha}, \tag{3.1}$$

and

$$\|I\|\le\begin{cases} c\tau^{l+1}\left|z\right|^{m-\alpha}+c\tau^k|z|^{k+m-l-1-\alpha}, & l=0\text{ or }l=1,3,\ldots,2k-1,\\ c\tau^{l+2}\left|z\right|^{m+1-\alpha}+c\tau^k|z|^{k+m-l-1-\alpha}, & l=2,4,\ldots,2k. \end{cases}$$

According to Lemma 3.1, (3.1), and the identity

$$\begin{aligned}&\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-A\right)^{-1}-(z^{\alpha}-A)^{-1}\\&\quad=\left(z^{\alpha}-\delta_{\tau,k}^{\alpha}(e^{-z\tau})\right)\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-A\right)^{-1}(z^{\alpha}-A)^{-1},\end{aligned}\tag{3.2}$$

we estimate II as

$$\|II\|\le c\tau^{k}|z|^{k+\alpha}c|z|^{-\alpha}c|z|^{-\alpha}|z|^{-l+m-1}\le c\tau^{k}|z|^{k+m-l-1-\alpha}.$$

Then the desired result is obtained. ∎

LEMMA 3.5. *Let $\delta_{\tau,k}^{\alpha}$ be given in (2.6), and let $\gamma_m(\xi)=\sum_{n=1}^{\infty}n^m\xi^n$ with $1\le m\le k\le 6$. Then there exists a positive constant c such that*

$$\|\mathcal{K}(z)\|\le\begin{cases}c\tau^{m+1}|z|^{m}+c\tau^{k}|z|^{k-1}, & m=1,3,5,\\ c\tau^{m+2}|z|^{m+1}+c\tau^{k}|z|^{k-1}, & m=2,4,6,\end{cases}$$

with

$$\mathcal{K}(z)=\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-A\right)^{-1}\delta_{\tau,k}^{m}(e^{-z\tau})\frac{\gamma_m(e^{-z\tau})}{m!}\tau^{m+1}A-(z^{\alpha}-A)^{-1}z^{-1}A.$$

Proof. Since $(z^{\alpha}-A)^{-1}z^{-1}A=-z^{-1}+(z^{\alpha}-A)^{-1}z^{\alpha}z^{-1}$ and

$$\begin{aligned}&\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-A\right)^{-1}\delta_{\tau,k}^{m}(e^{-z\tau})\frac{\gamma_m(e^{-z\tau})}{m!}\tau^{m+1}A\\&=\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-A\right)^{-1}\delta_{\tau,k}^{\alpha}(e^{-z\tau})\delta_{\tau,k}^{m}(e^{-z\tau})\frac{\gamma_m(e^{-z\tau})}{m!}\tau^{m+1}-\delta_{\tau,k}^{m}(e^{-z\tau})\frac{\gamma_m(e^{-z\tau})}{m!}\tau^{m+1},\end{aligned}$$

we can split $\mathcal{K}(z)$ as

$$\mathcal{K}(z)=J_1+J_2+J_3+J_4$$

with

$$\begin{aligned}&J_1=\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-A\right)^{-1}\delta_{\tau,k}^{\alpha}(e^{-z\tau})\left(\delta_{\tau,k}^{m}(e^{-z\tau})\frac{\gamma_m(e^{-z\tau})}{m!}\tau^{m+1}-z^{-1}\right),\\&J_2=\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-A\right)^{-1}\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-z^{\alpha}\right)z^{-1},\\&J_3=\left(\left(\delta_{\tau,k}^{\alpha}(e^{-z\tau})-A\right)^{-1}-(z^{\alpha}-A)^{-1}\right)z^{\alpha-1},\ J_4=z^{-1}-\delta_{\tau,k}^{m}(e^{-z\tau})\frac{\gamma_m(e^{-z\tau})}{m!}\tau^{m+1}.\end{aligned}$$

From (3.1), (3.2), and Lemmas 3.1 and 3.3, we estimate J_1, J_4 and J_2, J_3 as follows:

$$\|J_1\|\le c\,\|J_4\|\le\begin{cases}c\tau^{m+1}|z|^{m}+c\tau^{k}|z|^{k-1}, & m=1,3,5,\\ c\tau^{m+2}|z|^{m+1}+c\tau^{k}|z|^{k-1}, & m=2,4,6,\end{cases}$$

and

$$\|J_2\|\le c|z|^{-\alpha}\tau^{k}|z|^{k+\alpha}|z|^{-1}\le c\tau^{k}|z|^{k-1},\quad \|J_3\|\le c\tau^{k}|z|^{k-1}.$$

The proof is completed. ∎

3.2. Error analysis for general source function $g(t)$. Let $G(t) = J^m g(t)$, $1 \le m \le k \le 6$, be defined by (2.3). The Taylor expansion of the general source function with the remainder term in integral form is given by

$$\begin{aligned} \frac{t^{m-1}}{(m-1)!} * g(t) = G(t) &= \sum_{l=0}^{k+m-1} \frac{t^l}{l!} G^{(l)}(0) + \frac{t^{k+m-1}}{(k+m-1)!} * G^{(k+m)}(t) \\ &= \sum_{l=0}^{k+m-1} \frac{t^l}{l!} g^{(l-m)}(0) + \frac{t^{k+m-1}}{(k+m-1)!} * g^{(k)}(t) \end{aligned} \tag{3.3}$$

with $g^{(-i)}(0) = J^i g(0) = 0$, $i \ge 1$. Then we obtain the following results.

LEMMA 3.6. *Let $V(t_n)$ and V^n be the solutions of (2.4) and (2.7), respectively. Let $v = 0$ and $G(t) := \frac{t^l}{l!} g^{(l-m)}(0)$ with $l = 0, 1, \ldots, k+m-1$, $1 \le m \le k \le 6$. Then the following error estimate holds for any $t_n > 0$:*

$$\begin{aligned} &\|V(t_n) - V^n\|_{L^2(\Omega)} \\ &\quad \le \begin{cases} \left(c\tau^{l+1} t_n^{\alpha-m-1} + c\tau^k t_n^{\alpha+l-k-m}\right) \left\| g^{(l-m)}(0) \right\|_{L^2(\Omega)}, & l = 0, 1, 3, 5, \ldots, \\ \left(c\tau^{l+2} t_n^{\alpha-m-2} + c\tau^k t_n^{\alpha+l-k-m}\right) \left\| g^{(l-m)}(0) \right\|_{L^2(\Omega)}, & l = 2, 4, 6, \ldots. \end{cases} \end{aligned}$$

Proof. From (2.8) and Lemma 2.1, we have

$$V(t_n) = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}} e^{zt_n} (z^\alpha - A)^{-1} \frac{1}{z^{l+1-m}} g^{(l-m)}(0) dz,$$

and

$$V^n = \frac{1}{2\pi i} \int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n} \left(\delta^\alpha_{\tau,k}(e^{-z\tau}) - A\right)^{-1} \delta^m_{\tau,k}(e^{-z\tau}) \frac{\gamma_l(e^{-z\tau})}{l!} \tau^{l+1} g^{(l-m)}(0) dz$$

with $\gamma_l(\xi) = \sum_{n=1}^\infty n^l \xi^n$. Then we have

$$V(t_n) - V^n = J_1 + J_2$$

with

$$J_1 = \frac{1}{2\pi i} \int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n} K(z) g^{(l-m)}(0) dz, \ K(z) \text{ in Lemma 3.4},$$

and

$$J_2 = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa} \setminus \Gamma^\tau_{\theta,\kappa}} e^{zt_n} \left(z^\alpha - A\right)^{-1} \frac{1}{z^{l+1-m}} g^{(l-m)}(0) dz.$$

According to the triangle inequality, (2.2), and Lemma 3.4, this yields

$$\begin{aligned} \|J_1\|_{L^2(\Omega)} \le\, & c \int_\kappa^{\frac{\pi}{\tau \sin\theta}} e^{rt_n \cos\theta} \left(\tau^{l+1} r^{m-\alpha} + \tau^k r^{k+m-1-l-\alpha}\right) dr \left\| g^{(l-m)}(0) \right\|_{L^2(\Omega)} \\ & + c \int_{-\theta}^{\theta} e^{\kappa t_n \cos\psi} \left(\tau^{l+1} \kappa^{m+1-\alpha} + \tau^k \kappa^{k+m-l-\alpha}\right) d\psi \left\| g^{(l-m)}(0) \right\|_{L^2(\Omega)} \\ \le\, & \left(c\tau^{l+1} t_n^{\alpha-m-1} + c\tau^k t_n^{\alpha+l-k-m}\right) \left\| g^{(l-m)}(0) \right\|_{L^2(\Omega)}, \ l = 0 \text{ or } l = 1, 3, \ldots, \end{aligned}$$

and

$$\|J_1\|_{L^2(\Omega)} \leq \left(c\tau^{l+2}t_n^{\alpha-m-2} + c\tau^k t_n^{\alpha+l-k-m}\right)\left\|g^{(l-m)}(0)\right\|_{L^2(\Omega)}, \quad l=2,4,\ldots,$$

where we use

$$\begin{aligned} &\int_{\kappa}^{\frac{\pi}{\tau\sin\theta}} e^{rt_n\cos\theta}r^{k+m-1-l-\alpha}dr \leq ct_n^{\alpha+l-k-m}, \\ &\int_{-\theta}^{\theta} e^{\kappa t_n\cos\psi}\kappa^{k+m-l-\alpha}d\psi \leq ct_n^{\alpha+l-k-m}. \end{aligned} \tag{3.4}$$

From (2.2), one has

$$\begin{aligned} \|J_2\|_{L^2(\Omega)} &\leq c\int_{\frac{\pi}{\tau\sin\theta}}^{\infty} e^{rt_n\cos\theta}r^{m-l-1-\alpha}dr\left\|g^{(l-m)}(0)\right\|_{L^2(\Omega)} \\ &\leq c\tau^k\int_{\frac{\pi}{\tau\sin\theta}}^{\infty} e^{rt_n\cos\theta}r^{k+m-1-l-\alpha}dr\left\|g^{(l-m)}(0)\right\|_{L^2(\Omega)} \\ &\leq c\tau^k t_n^{\alpha+l-k-m}\left\|g^{(l-m)}(0)\right\|_{L^2(\Omega)}. \end{aligned}$$

Here we use $1 \leq (\frac{\sin\theta}{\pi})^k\tau^k r^k$ with $r \geq \frac{\pi}{\tau\sin\theta}$. The proof is completed. ∎

LEMMA 3.7. *Let $V(t_n)$ and V^n be the solutions of (2.4) and (2.7), respectively. Let $v=0$, $G(t):=\frac{t^{k+m-1}}{(k+m-1)!}*g^{(k)}(t)$, $1\leq m\leq k\leq 6$, and $\int_0^t(t-s)^{\alpha-1}\|g^{(k)}(s)\|_{L^2(\Omega)}ds<\infty$. Then the following error estimate holds for any $t_n>0$:*

$$\|V(t_n)-V^n\|_{L^2(\Omega)} \leq c\tau^k\int_0^{t_n}(t_n-s)^{\alpha-1}\left\|g^{(k)}(s)\right\|_{L^2(\Omega)}ds.$$

Proof. From the continuous solution representation in (2.8), we have

$$V(t_n) = (\mathscr{E}(t)*G(t))(t_n) = \left(\left(\mathscr{E}(t)*\frac{t^{k+m-1}}{(k+m-1)!}\right)*g^{(k)}(t)\right)(t_n) \tag{3.5}$$

with

$$\mathscr{E}(t) = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{zt}(z^\alpha - A)^{-1}z^m dz. \tag{3.6}$$

Let $\sum_{n=0}^{\infty}\mathscr{E}_\tau^n\xi^n = \widetilde{\mathscr{E}_\tau}(\xi) := (\delta_{\tau,k}^{\alpha}(\xi)-A)^{-1}\delta_{\tau,k}^{m}(\xi)$. Then using (2.10), this yields

$$\begin{aligned} \widetilde{V}(\xi) &= \left(\delta_{\tau,k}^{\alpha}(\xi)-A\right)^{-1}\delta_{\tau,k}^{m}(\xi)\widetilde{G}(\xi) = \widetilde{\mathscr{E}_\tau}(\xi)\widetilde{G}(\xi) = \sum_{n=0}^{\infty}\mathscr{E}_\tau^n\xi^n\sum_{j=0}^{\infty}G^j\xi^j \\ &= \sum_{n=0}^{\infty}\sum_{j=0}^{\infty}\mathscr{E}_\tau^n G^j\xi^{n+j} = \sum_{j=0}^{\infty}\sum_{n=j}^{\infty}\mathscr{E}_\tau^{n-j}G^j\xi^n = \sum_{n=0}^{\infty}\sum_{j=0}^{n}\mathscr{E}_\tau^{n-j}G^j\xi^n = \sum_{n=0}^{\infty}V^n\xi^n \end{aligned}$$

with

$$V^n = \sum_{j=0}^{n}\mathscr{E}_\tau^{n-j}G^j := \sum_{j=0}^{n}\mathscr{E}_\tau^{n-j}G(t_j).$$

According to Cauchy's integral formula and the change of variables $\xi = e^{-z\tau}$, we get the representation of the $\mathscr{E}_\tau^n$ as follows:

$$\mathscr{E}_\tau^n = \frac{1}{2\pi i}\int_{|\xi|=\rho} \xi^{-n-1}\widetilde{\mathscr{E}_\tau}(\xi)d\xi = \frac{\tau}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\left(\delta_{\tau,k}^\alpha(e^{-z\tau}) - A\right)^{-1}\delta_{\tau,k}^m(e^{-z\tau})dz.$$

From (3.1), Lemma 3.1, and $\tau t_n^{-1} = \frac{1}{n} \le 1$, this implies

$$\|\mathscr{E}_\tau^n\| \le c\tau\left(\int_\kappa^{\frac{\pi}{\tau\sin\theta}} e^{rt_n\cos\theta}r^{m-\alpha}dr + \int_{-\theta}^{\theta} e^{\kappa t_n\cos\psi}\kappa^{m+1-\alpha}d\psi\right) \le ct_n^{\alpha-m}. \tag{3.7}$$

Let $\mathscr{E}_\tau(t) = \sum_{n=0}^\infty \mathscr{E}_\tau^n\delta_{t_n}(t)$, with δ_{t_n} being the Dirac delta function at t_n. Then

$$\begin{aligned}(\mathscr{E}_\tau(t) * G(t))(t_n) &= \left(\sum_{j=0}^\infty \mathscr{E}_\tau^j\delta_{t_j}(t) * G(t)\right)(t_n)\\ &= \sum_{j=0}^n \mathscr{E}_\tau^j G(t_n - t_j) = \sum_{j=0}^n \mathscr{E}_\tau^{n-j}G(t_j) = V^n.\end{aligned} \tag{3.8}$$

Moreover, using the above equation, there exists

$$\begin{aligned}(\widetilde{\mathscr{E}_\tau * t^l})(\xi) &= \sum_{n=0}^\infty\sum_{j=0}^n \mathscr{E}_\tau^{n-j}t_j^l\xi^n = \sum_{j=0}^\infty\sum_{n=j}^\infty \mathscr{E}_\tau^{n-j}t_j^l\xi^n = \sum_{j=0}^\infty\sum_{n=0}^\infty \mathscr{E}_\tau^n t_j^l\xi^{n+j}\\ &= \sum_{n=0}^\infty \mathscr{E}_\tau^n\xi^n\sum_{j=0}^\infty t_j^l\xi^j = \widetilde{\mathscr{E}_\tau}(\xi)\tau^l\sum_{j=0}^\infty j^l\xi^j = \widetilde{\mathscr{E}_\tau}(\xi)\tau^l\gamma_l(\xi).\end{aligned}$$

Combining (3.5), (3.8), and Lemma 3.6, we have

$$\left\|\left((\mathscr{E}_\tau - \mathscr{E}) * \frac{t^l}{l!}\right)(t_n)\right\| \le \begin{cases} c\tau^{l+1}t_n^{\alpha-m-1} + c\tau^k t_n^{\alpha+l-k-m}, & l = 0,1,3,\ldots,\\[2mm] c\tau^{l+2}t_n^{\alpha-m-2} + c\tau^k t_n^{\alpha+l-k-m}, & l = 2,4,6,\ldots,\end{cases} \tag{3.9}$$

with $l \le k+m-1$.

Next, we prove the following inequality (3.10) for $t > 0$:

$$\left\|\left((\mathscr{E}_\tau - \mathscr{E}) * \frac{t^{k+m-1}}{(k+m-1)!}\right)(t)\right\| \le c\tau^k t^{\alpha-1} \quad \forall t \in (t_{n-1}, t_n). \tag{3.10}$$

Applying the Taylor series expansion of $\mathscr{E}(t)$ at $t = t_n$, we get

$$\begin{aligned}\left(\mathscr{E} * \frac{t^{k+m-1}}{(k+m-1)!}\right)(t) = &\sum_{l=0}^{k+m-1}\frac{(t-t_n)^l}{l!}\left(\mathscr{E} * \frac{t^{k+m-l-1}}{(k+m-l-1)!}\right)(t_n)\\ &+ \frac{1}{(k+m-1)!}\int_{t_n}^t (t-s)^{k+m-1}\mathscr{E}(s)ds,\end{aligned}$$

which also holds for the convolution $\left(\mathscr{E}_\tau * t^{k+m-1}\right)(t)$. From (3.9), this leads to

$$\begin{aligned}\left\|(t-t_n)^l\left((\mathscr{E}_\tau - \mathscr{E}) * t^{k+m-l-1}\right)(t_n)\right\| &\le c\tau^l\left(\tau^{k+m-l}t_n^{\alpha-m-1} + \tau^k t_n^{\alpha-l-1}\right)\\ &\le c\tau^k t^{\alpha-1} \quad \forall t \in (t_{n-1}, t_n).\end{aligned}$$

According to (3.6), (2.2), and (3.4), one has

$$\|\mathscr{E}(t)\| \leq c\left(\int_\kappa^\infty e^{rt\cos\theta} r^{m-\alpha} dr + \int_{-\theta}^{\theta} e^{\kappa t\cos\psi}\kappa^{m+1-\alpha} d\psi\right) \leq ct^{\alpha-m-1}.$$

Moreover, we get

$$\left\|\int_{t_n}^t (t-s)^{k+m-1}\mathscr{E}(s)ds\right\| \leq c\int_t^{t_n}(s-t)^{k+m-1}s^{\alpha-m-1}ds \leq c\tau^k t^{\alpha-1}.$$

By the definition of $\mathscr{E}_\tau(t) = \sum_{n=0}^\infty \mathscr{E}_\tau^n \delta_{t_n}(t)$ in (3.8) and (3.7), we deduce

$$\begin{aligned}\left\|\int_{t_n}^t (t-s)^{k+m-1}\mathscr{E}_\tau(s)ds\right\| &\leq (t_n-t)^{k+m-1}\|\mathscr{E}_\tau^n\| \leq c\tau^{k+m}t_n^{\alpha-m-1}\\ &\leq c\tau^k t_n^{\alpha-1} \leq c\tau^k t^{\alpha-1} \quad \forall t\in(t_{n-1},t_n).\end{aligned}$$

Using the above inequalities, we obtain (3.10). The proof is completed. ∎

For simplicity, we take

$$\|J_v\|_{L^2(\Omega)} = \begin{cases} c\tau^{m+1}t_n^{-m-1}\|v\|_{L^2(\Omega)} + c\tau^k t_n^{-k}\|v\|_{L^2(\Omega)}, & m=1,3,5,\\ c\tau^{m+2}t_n^{-m-2}\|v\|_{L^2(\Omega)} + c\tau^k t_n^{-k}\|v\|_{L^2(\Omega)}, & m=2,4,6,\end{cases} \tag{3.11}$$

and

$$\|J_g\|_{L^2(\Omega)} = \begin{cases} c\sum_{l=0}^{k-1}\left(\tau^{l+m+1}t_n^{\alpha-m-1}+\tau^k t_n^{\alpha+l-k}\right)\left\|g^{(l)}(0)\right\|_{L^2(\Omega)}, & l+m=1,3,5,\ldots,\\ c\sum_{l=0}^{k-1}\left(\tau^{l+m+2}t_n^{\alpha-m-2}+\tau^k t_n^{\alpha+l-k}\right)\left\|g^{(l)}(0)\right\|_{L^2(\Omega)}, & l+m=2,4,6,\ldots.\end{cases}$$

Then we have the following result.

THEOREM 3.8. *Let $V(t_n)$ and V^n be the solutions of* (2.4) *and* (2.7), *respectively. Let $v\in L^2(\Omega)$, $g\in C^{k-1}([0,T];L^2(\Omega))$, and $\int_0^t (t-s)^{\alpha-1}\left\|g^{(k)}(s)\right\|_{L^2(\Omega)}ds<\infty$. Then the following error estimate holds for any $t_n>0$:*

$$\|V^n - V(t_n)\|_{L^2(\Omega)} \leq ||J_v||_{L^2(\Omega)} + ||J_g||_{L^2(\Omega)} + c\tau^k\int_0^{t_n}(t_n-s)^{\alpha-1}\left\|g^{(k)}(s)\right\|_{L^2(\Omega)}ds.$$

Proof. Subtracting (2.8) from (2.11), we obtain

$$V^n - V(t_n) = I_1 - I_2 + I_3$$

with the related initial terms

$$\begin{aligned} I_1 &= \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\mathcal{K}(z)vdz, \ \mathcal{K}(z) \text{ in Lemma 3.5},\\ I_2 &= \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}\setminus\Gamma_{\theta,\kappa}^\tau} e^{zt_n}(z^\alpha - A)^{-1}z^{-1}Avdz,\end{aligned} \tag{3.12}$$

and the related source term

$$\begin{aligned} I_3 = &\frac{\tau}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\left(\delta_{\tau,k}^\alpha(e^{-z\tau})-A\right)^{-1}\delta_{\tau,k}^m(e^{-z\tau})\widetilde{G}(e^{-z\tau})dz\\ &-\frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{zt_n}(z^\alpha - A)^{-1}z^m\widehat{G}(z)dz.\end{aligned}$$

Similarly to the manner in Lemma 3.6, we estimate

$$\|I_1\|_{L^2(\Omega)} \leq \begin{cases} c\tau^{m+1}t_n^{-m-1}\|v\|_{L^2(\Omega)} + c\tau^k t_n^{-k}\|v\|_{L^2(\Omega)}, & m=1,3,5, \\ c\tau^{m+2}t_n^{-m-2}\|v\|_{L^2(\Omega)} + c\tau^k t_n^{-k}\|v\|_{L^2(\Omega)}, & m=2,4,6. \end{cases} \tag{3.13}$$

Using the resolvent estimate (2.2), we estimate the second term I_2 as follows:

$$\|I_2\|_{L^2(\Omega)} \leq c\int_{\Gamma_{\theta,\kappa}\setminus\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right| |z|^{-1}\|v\|_{L^2(\Omega)}|dz| \leq c\tau^k t_n^{-k}\|v\|_{L^2(\Omega)}, \tag{3.14}$$

since

$$\int_{\Gamma_{\theta,\kappa}\setminus\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right| |z|^{-1}|dz| = \int_{\frac{\pi}{\tau\sin\theta}}^\infty e^{rt_n\cos\theta}r^{-1}dr \leq c\tau^k t_n^{-k} \tag{3.15}$$

with $1 \leq (\frac{\sin\theta}{\pi})^k\tau^k r^k$, $r\tau \geq \frac{\pi}{\sin\theta}$. Then we have $\|I_1\|_{L^2(\Omega)} + \|I_2\|_{L^2(\Omega)} \leq \|J_v\|_{L^2(\Omega)}$.

According to Lemmas 3.6 and 3.7 and the general source function (3.3), i.e.,

$$G(t) = \sum_{l=0}^{k-1} \frac{t^{(l+m)}}{(l+m)!}g^{(l)}(0) + \frac{t^{k+m-1}}{(k+m-1)!} * g^{(k)}(t),$$

we have $\|I_3\|_{L^2(\Omega)} \leq \|J_g\|_{L^2(\Omega)} + c\tau^k\int_0^{t_n}(t_n-s)^{\alpha-1}\left\|g^{(k)}(s)\right\|_{L^2(\Omega)}ds$. The proof is completed. ∎

4. Convergence analysis: Singular source function $t^\mu q$, $\mu > -1$.

We next consider the singular source term $g(t) = t^\mu q$ with $\mu > -1$ for (2.4). We introduce the polylogarithm function

$$Li_p(\xi) = \sum_{j=1}^\infty \frac{\xi^j}{j^p}, \quad p \notin \mathbb{N}, \tag{4.1}$$

with the Riemann zeta function $\zeta(p) = Li_p(1)$.

Let $G(t) = J^m g(t) = \frac{\Gamma(\mu+1)t^{\mu+m}}{\Gamma(\mu+m+1)}q$ with the Laplace transform $\widehat{G}(z) = \frac{\Gamma(\mu+1)}{z^{\mu+m+1}}q$. From (2.8) and (2.11), this yields the continuous solution

$$V(t) = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{zt}(z^\alpha - A)^{-1}\left(z^{-1}Av + \frac{\Gamma(\mu+1)}{z^{\mu+1}}q\right)dz$$

and the discrete solution

$$V^n = \frac{\tau}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}(\delta_{\tau,k}^\alpha(e^{-z\tau}) - A)^{-1}\delta_{\tau,k}^m(e^{-z\tau})\left(\frac{\gamma_m(e^{-z\tau})}{m!}\tau^m Av + \widetilde{G}(e^{-z\tau})\right)dz$$

with

$$\widetilde{G}(\xi) = \sum_{n=1}^\infty G^n\xi^n = q\frac{\Gamma(\mu+1)\tau^{\mu+m}\sum_{n=1}^\infty n^{\mu+m}\xi^n}{\Gamma(\mu+m+1)} = q\frac{\Gamma(\mu+1)\tau^{\mu+m}Li_{-\mu-m}(\xi)}{\Gamma(\mu+m+1)}.$$

LEMMA 4.1 (see [11]). *Let $|z\tau| \leq \frac{\pi}{\sin\theta}$ and $\theta > \pi/2$ be close to $\pi/2$. Then we have*

$$Li_p(e^{-z\tau}) = \Gamma(1-p)(z\tau)^{p-1} + \sum_{j=0}^\infty(-1)^j\zeta(p-j)\frac{(z\tau)^j}{j!}, \quad p \notin \mathbb{N},$$

and the infinite series converges absolutely. Here ζ denotes the Riemann zeta function.

LEMMA 4.2. *Let $\gamma_{\mu+m}(\xi)=\sum_{n=1}^{\infty} n^{\mu+m}\xi^n$ with $1\le m\le k\le 6$. Then there exists a positive constant c such that*

$$\left|\frac{\gamma_{\mu+m}(e^{-z\tau})}{\Gamma(\mu+m+1)}\tau^{\mu+m+1}-\frac{1}{z^{\mu+m+1}}\right|\le c\tau^{\mu+m+1},\quad \mu>-1.$$

Proof. From Lemma 3.2, the desired result is obtained with $\mu\in\mathbb{N}$. We next prove the case $\mu\notin\mathbb{N}$. Using (4.1) and Lemma 4.1, we obtain

$$\begin{aligned}&\left|\frac{\gamma_{\mu+m}(e^{-z\tau})}{\Gamma(\mu+m+1)}\tau^{\mu+m+1}-\frac{1}{z^{\mu+m+1}}\right|\\ &=\left|\frac{\tau^{\mu+m+1}}{\Gamma(\mu+m+1)}\left(Li_{-\mu-m}(e^{-z\tau})-\frac{\Gamma(\mu+m+1)}{(z\tau)^{\mu+m+1}}\right)\right|\\ &\le\frac{\tau^{\mu+m+1}}{\Gamma(\mu+m+1)}\left|\sum_{j=0}^{\infty}(-1)^j\zeta(-\mu-m-j)\frac{(z\tau)^j}{j!}\right|\le c\tau^{\mu+m+1}.\end{aligned}$$

The proof is completed. ◻

LEMMA 4.3. *Let $\delta_{\tau,k}(\xi)$ with $k\le 6$ be given in (2.6). Then there exists a positive constant c such that*

$$\left\|\left(\delta^{\alpha}_{\tau,k}(e^{-z\tau})-A\right)^{-1}\delta^{m}_{\tau,k}(e^{-z\tau})-(z^{\alpha}-A)^{-1}z^m\right\|\le c\tau^k|z|^{k+m-\alpha}\quad\forall z\in\Gamma^{\tau}_{\theta,\kappa}.$$

Proof. Let

$$\left(\delta^{\alpha}_{\tau,k}(e^{-z\tau})-A\right)^{-1}\delta^{m}_{\tau,k}(e^{-z\tau})-(z^{\alpha}-A)^{-1}z^m=I+II$$

with

$$\begin{aligned}I&=\left(\delta^{\alpha}_{\tau,k}(e^{-z\tau})-A\right)^{-1}\left(\delta^{m}_{\tau,k}(e^{-z\tau})-z^m\right),\\ II&=\left(\left(\delta^{\alpha}_{\tau,k}(e^{-z\tau})-A\right)^{-1}-(z^{\alpha}-A)^{-1}\right)z^m.\end{aligned}$$

From (3.1) and Lemma 3.1, we obtain

$$\|I\|\le c\tau^k|z|^{k+m-\alpha}.$$

Using Lemma 3.1, (3.1), (2.2), and the identity

$$\left(\delta^{\alpha}_{\tau,k}(e^{-z\tau})-A\right)^{-1}-(z^{\alpha}-A)^{-1}=\left(z^{\alpha}-\delta^{\alpha}_{\tau,k}(e^{-z\tau})\right)\left(\delta^{\alpha}_{\tau,k}(e^{-z\tau})-A\right)^{-1}(z^{\alpha}-A)^{-1},$$

we estimate II as follows:

$$\|II\|\le c\tau^k|z|^{k+\alpha}c|z|^{-\alpha}c|z|^{-\alpha}|z|^m\le c\tau^k|z|^{k+m-\alpha}.$$

According to the triangle inequality, the desired result is obtained. ◻

THEOREM 4.4. *Let $V(t_n)$ and V^n be the solutions of (2.4) and (2.7), respectively. Let $v\in L^2(\Omega)$ and $g(x,t)=t^{\mu}q$, $\mu>-1$, $q\in L^2(\Omega)$. Then the following error estimate holds for any $t_n>0$:*

$$\|V^n-V(t_n)\|_{L^2(\Omega)}\le\|J_v\|_{L^2(\Omega)}+c\tau^{\mu+m+1}t_n^{\alpha-m-1}\|q\|_{L^2(\Omega)}+c\tau^k t_n^{\alpha+\mu-k}\|q\|_{L^2(\Omega)}$$

with $\|J_v\|_{L^2(\Omega)}$ in (3.11).

Proof. From Theorem 3.8, the desired result is obtained with $\mu \in \mathbb{N}$. We next prove the case $\mu \notin \mathbb{N}$. Subtracting (2.8) from (2.11), we obtain

$$V^n - V(t_n) = I_1 - I_2 + I_3 - I_4,$$

where I_1, I_2 are defined by (3.12), and

$$\begin{aligned} I_3 =& \frac{1}{2\pi i}\int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n}\left[\left(\delta^\alpha_{\tau,k}(e^{-z\tau})-A\right)^{-1}\delta^m_{\tau,k}(e^{-z\tau})\tau\widetilde{G}(e^{-z\tau}) - (z^\alpha - A)^{-1}z^m\widehat{G}(z)\right]dz,\\ I_4 =& \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}\setminus\Gamma^\tau_{\theta,\kappa}} e^{zt_n}(z^\alpha - A)^{-1}z^m\widehat{G}(z)dz. \end{aligned}$$

According to (3.13) and (3.14), we estimate $\|I_1\|_{L^2(\Omega)} + \|I_2\|_{L^2(\Omega)} \le \|J_v\|_{L^2(\Omega)}$. From (3.15), this leads to

$$\|I_4\|_{L^2(\Omega)} \le c\int_{\Gamma_{\theta,\kappa}\setminus\Gamma^\tau_{\theta,\kappa}} \left|e^{zt_n}\right||z|^{-\alpha}|z|^{-\mu-1}\|q\|_{L^2(\Omega)}|dz| \le c\tau^k t_n^{\alpha+\mu-k}\|q\|_{L^2(\Omega)}.$$

Finally we consider $I_3 = I_{31} + I_{32}$ with

$$\begin{aligned} I_{31} =& \frac{1}{2\pi i}\int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n}\left(\delta^\alpha_{\tau,k}(e^{-z\tau})-A\right)^{-1}\delta^m_{\tau,k}(e^{-z\tau})\left(\tau\widetilde{G}(e^{-z\tau}) - \widehat{G}(z)\right)dz,\\ I_{32} =& \frac{1}{2\pi i}\int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n}\left(\left(\delta^\alpha_{\tau,k}(e^{-z\tau})-A\right)^{-1}\delta^m_{\tau,k}(e^{-z\tau}) - (z^\alpha - A)^{-1}z^m\right)\widehat{G}(z)dz. \end{aligned}$$

According to (3.1) and Lemmas 3.1 and 4.2, there exists

$$\|I_{31}\|_{L^2(\Omega)} \le c\tau^{\mu+m+1}\|q\|_{L^2(\Omega)}\int_{\Gamma^\tau_{\theta,\kappa}}\left|e^{zt_n}\right||z|^{m-\alpha}|dz| \le c\tau^{\mu+m+1}t_n^{\alpha-m-1}\|q\|_{L^2(\Omega)}.$$

From Lemma 4.3 and $\widehat{G}(z) = \frac{\Gamma(\mu+1)}{z^{\mu+m+1}}q$, we have

$$\|I_{32}\|_{L^2(\Omega)} \le c\tau^k\|q\|_{L^2(\Omega)}\int_{\Gamma^\tau_{\theta,\kappa}}\left|e^{zt_n}\right||z|^{k+m-\alpha}|z|^{-\mu-m-1}|dz| \le c\tau^k t_n^{\alpha+\mu-k}\|q\|_{L^2(\Omega)}.$$

The proof is completed. ∎

5. Convergence analysis: Source function $t^\mu \circ f(t)$ with $\mu > -1$.

Based on the analysis of sections 3 and 4, we next provide the detailed error estimates for the model (1.1) with the singular/low regularity source function $t^\mu \circ f(t)$.

5.1. Convergence analysis: Convolution source function $t^\mu * f(t)$, $\mu > -1$.

Let $f(t) = \sum_{j=0}^{k-1}\frac{t^j}{j!}f^{(j)}(0) + \frac{t^{k-1}}{(k-1)!} * f^{(k)}(t)$. Then we obtain

$$g(t) = t^\mu * f(t) = \sum_{j=0}^{k-1}\frac{\Gamma(\mu+1)t^{\mu+j+1}}{\Gamma(\mu+j+2)}f^{(j)}(0) + t^\mu * \frac{t^{k-1}}{(k-1)!} * f^{(k)}(t).$$

Let $G(t) = J^m g(t) = \frac{\Gamma(\mu+1)t^{\mu+m}}{\Gamma(\mu+m+1)} * f(t)$ with $G^{(j)}(0) = 0,\ j = 0,\ldots,m-1$. This yields

$$G(t) = \sum_{j=0}^{k-1}\frac{\Gamma(\mu+1)t^{\mu+j+m+1}}{\Gamma(\mu+j+m+2)}f^{(j)}(0) + \frac{t^{k+m-1}}{(k+m-1)!} * t^\mu * f^{(k)}(t).$$

LEMMA 5.1. *Let $V(t_n)$ and V^n be the solutions of* (2.4) *and* (2.7)*, respectively. Let $v=0$, $G(t):=\frac{t^{k+m-1}}{(k+m-1)!}*\left(t^\mu * f^{(k)}(t)\right)$ with $\mu>-1$ and $\int_0^t (t-s)^{\alpha-1}s^\mu * \left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds<\infty$. Then the following error estimate holds for any $t_n>0$:*

$$\begin{aligned}\|V(t_n)-V^n\|_{L^2(\Omega)} &\le c\tau^k\int_0^{t_n}(t_n-s)^{\alpha-1}s^\mu * \left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds\\ &\le c\tau^k\int_0^{t_n}(t_n-s)^{\alpha+\mu}\left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds.\end{aligned}$$

Proof. From Lemma 3.7 and $g^{(k)}(t)=t^\mu * f^{(k)}(t)$, we obtain

$$\begin{aligned}\|V(t_n)-V^n\|_{L^2(\Omega)} &\le c\tau^k\int_0^{t_n}(t_n-s)^{\alpha-1}\left\|s^\mu * f^{(k)}(s)\right\|_{L^2(\Omega)}ds\\ &\le c\tau^k\int_0^{t_n}(t_n-s)^{\alpha-1}s^\mu * \left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds\\ &= c\tau^k\left(\left(t^{\alpha-1}*t^\mu\right)*\left\|f^{(k)}(t)\right\|_{L^2(\Omega)}\right)_{t=t_n}\\ &\le c\tau^k\int_0^{t_n}(t_n-s)^{\alpha+\mu}\left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds.\end{aligned}$$

The proof is completed. ◻

THEOREM 5.2. *Let $V(t_n)$ and V^n be the solutions of* (2.4) *and* (2.7)*, respectively. Let $v\in L^2(\Omega)$, $g(t)=t^\mu * f(t)$, $\mu>-1$, and $f\in C^{k-1}([0,T];L^2(\Omega))$, $\int_0^t(t-s)^{\alpha-1}s^\mu * \left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds<\infty$. Then the following error estimate holds for any $t_n>0$:*

$$\begin{aligned}\|V^n-V(t_n)\|_{L^2(\Omega)} \le{}& \|J_v\|_{L^2(\Omega)}+c\tau^k\int_0^{t_n}(t_n-s)^{\alpha-1}s^\mu * \left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds\\ &+c\sum_{j=0}^{k-1}\left(\tau^{\mu+j+m+2}t_n^{\alpha-m-1}+\tau^k t_n^{\alpha+\mu+j-k+1}\right)\left\|f^{(j)}(0)\right\|_{L^2(\Omega)}\end{aligned}$$

with $\|J_v\|_{L^2(\Omega)}$ in (3.11).

Proof. From Theorem 4.4 and Lemma 5.1, the desired result is obtained. ◻

5.2. Convergence analysis: Product source function $t^\mu f(t)$, $\mu>-1$. Let $G(t)=J^m g(t)$ with $g(t)=t^\mu f(t)$, $f(t)=\sum_{j=0}^{k-1}\frac{t^j}{j!}f^{(j)}(0)+\frac{t^{k-1}}{(k-1)!}*f^{(k)}(t)$. Then

$$G(t)=\sum_{j=0}^{k-1}\frac{\Gamma(\mu+j+1)t^{\mu+j+m}}{\Gamma(\mu+j+m+1)j!}f^{(j)}(0)+\frac{t^{m-1}}{\Gamma(m)}*h(t)$$

with $h(t)=t^\mu(\frac{t^{k-1}}{(k-1)!}*f^{(k)}(t))$.

LEMMA 5.3. *Let $h(t)=t^\mu(\frac{t^{k-1}}{(k-1)!}*f^{(k)}(t))$ with $\mu>-1$ and*

$$f\in C^{k-1}([0,T];L^2(\Omega)),\ \int_0^t\left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds<\infty,\ \int_0^t s^\mu\left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds<\infty.$$

Then the following error estimate holds:

$$\left\|h^{(k-1)}(0)\right\|_{L^2(\Omega)}\le c\int_0^t s^\mu\left\|f^{(k)}(s)\right\|_{L^2(\Omega)}ds,\ \ h^{(l)}(0)=0\ \ \forall l\le k-2,\ 2\le k\le 6,$$

and

$$\left\|h^{(k-1)}(0)\right\|_{L^2(\Omega)} \leq c\int_0^t s^\mu \left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds,\ k=1.$$

Proof. Let us consider the case $\mu \notin \mathbb{N}$, since the result is trivial if $\mu \in \mathbb{N}$. Using Leibnitz's formula for the lth-order derivative of the function $h(t)$, we get

$$h^{(l)}(t) = \sum_{j=0}^{l} \binom{l}{j} \frac{\Gamma(\mu+1)}{\Gamma(\mu+1-j)} t^{\mu-j} \left(\frac{t^{k-1-l+j}}{\Gamma(k-l+j)} * f^{(k)}(t)\right)\ \forall l \leq k-1. \tag{5.1}$$

Case 1: $2 \leq k \leq 6$. From (5.1), we have

$$\begin{aligned}\left\|h^{(l)}(t)\right\|_{L^2(\Omega)} &\leq c\sum_{j=0}^{l} t^{\mu-j}\int_0^t s^{k-1-l+j}\left\|f^{(k)}(t-s)\right\|_{L^2(\Omega)} ds\\ &\leq c\sum_{j=0}^{l} t^{\mu-j}\int_0^t t^{k-1-l+j}\left\|f^{(k)}(t-s)\right\|_{L^2(\Omega)} ds \leq ct^{\mu+k-1-l}\ \ \forall l \leq k-2,\end{aligned}$$

and $h^{(l)}(0)=0\ \forall l \leq k-2,\ k \geq 2$.

We next estimate the bound of $h^{(k-1)}(0)$. From the above inequality, it implies $h^{(k-1)}(0)=0$ for $\mu>0$. For $-1<\mu<0$, using (5.1), we obtain

$$\begin{aligned}\left\|h^{(k-1)}(t)\right\|_{L^2(\Omega)} &\leq c\sum_{j=0}^{k-1} t^{\mu-j}\int_0^t t^j \left\|f^{(k)}(t-s)\right\|_{L^2(\Omega)} ds\\ &= c\sum_{j=0}^{k-1}\int_0^t t^\mu \left\|f^{(k)}(t-s)\right\|_{L^2(\Omega)} ds \leq c\int_0^t s^\mu \left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds.\end{aligned}$$

Case 2: $k=1$. From the above inequality, the desired result is obtained. ∎

LEMMA 5.4. *Let $V(t_n)$ and V^n be the solutions of* (2.4) *and* (2.7)*, respectively. Let $v=0$, $G(t)=\frac{t^{m-1}}{(m-1)!} * [t^\mu(\frac{t^{k-1}}{(k-1)!} * f^{(k)}(t))]$, $\mu>-1$, and $f \in C^{k-1}([0,T];L^2(\Omega))$ and*

$$\int_0^t \left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds < \infty,\ \int_0^t s^{\frac{\mu-1}{2}} \left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds < \infty,$$

and

$$\int_0^t (t-s)^{\alpha-1} s^\mu \left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds < \infty.$$

Then the following error estimate holds for any $t_n>0$:

$$\begin{aligned}&\|V(t_n)-V^n\|_{L^2(\Omega)}\\ &\leq c\tau^k\left(t_n^{\alpha+\mu-1}\int_0^{t_n}\left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds + t_n^{\alpha+\frac{\mu-1}{2}}\int_0^{t_n} s^{\frac{\mu-1}{2}}\left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds\right.\\ &\qquad\left.+\int_0^{t_n}(t_n-s)^{\alpha-1}s^\mu\left\|f^{(k)}(s)\right\|_{L^2(\Omega)} ds\right),\ \ \mu>-1.\end{aligned}$$

Proof. Let us consider the case $\mu \notin \mathbb{N}$, since the result is trivial if $\mu \in \mathbb{N}$. Let $h(t) = t^{\mu}(\frac{t^{k-1}}{(k-1)!} * f^{(k)}(t))$. From Lemma 5.3, we have

$$G(t) = \frac{t^{m-1}}{(m-1)!} * h(t) = \frac{t^{k+m-1}}{(k+m-1)!} h^{(k-1)}(0) + \frac{t^{k+m-1}}{(k+m-1)!} * h^{(k)}(t).$$

According to Theorem 4.4 and Lemma 3.7, this yields

$$\|V(t_n) - V^n\|_{L^2(\Omega)} \le c\tau^k \left(t_n^{\alpha-1} \left\| h^{(k-1)}(0) \right\|_{L^2(\Omega)} + \int_0^{t_n} (t_n - s)^{\alpha-1} \left\| h^{(k)}(s) \right\|_{L^2(\Omega)} ds \right)$$

with

$$h^{(k)}(t) = \sum_{j=1}^{k} \binom{k}{j} \frac{\Gamma(\mu+1)}{\Gamma(\mu+1-j)} t^{\mu-j} \left(\frac{t^{j-1}}{\Gamma(j)} * f^{(k)}(t) \right) + t^{\mu} f^{(k)}(t).$$

Since

$$\begin{aligned}
&\sum_{j=1}^{k} \int_0^{t_n} (t_n - s)^{\alpha-1} \left\| s^{\mu-j} \left(s^{j-1} * f^{(k)}(s) \right) \right\|_{L^2(\Omega)} ds \\
&\quad = \sum_{j=1}^{k} \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\frac{\mu-1}{2}} \left\| \int_0^s s^{\frac{\mu-1}{2}} \frac{(s-w)^{j-1}}{s^{j-1}} f^{(k)}(w) dw \right\|_{L^2(\Omega)} ds \\
&\quad \le k \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\frac{\mu-1}{2}} \int_0^{t_n} w^{\frac{\mu-1}{2}} \left\| f^{(k)}(w) \right\|_{L^2(\Omega)} dw ds \\
&\quad = kB(\alpha, (\mu+1)/2) t_n^{\alpha + \frac{\mu-1}{2}} \int_0^{t_n} w^{\frac{\mu-1}{2}} \left\| f^{(k)}(w) \right\|_{L^2(\Omega)} dw, \ -1 < \mu < 0,
\end{aligned}$$

where we use

$$\int_0^{t_n} (t_n - s)^{\alpha-1} s^{\frac{\mu-1}{2}} ds = t_n^{\alpha+\frac{\mu-1}{2}} \int_0^1 (1-s)^{\alpha-1} s^{\frac{\mu-1}{2}} ds = B\left(\alpha, \frac{\mu+1}{2}\right) t_n^{\alpha+\frac{\mu-1}{2}},$$

similarly, we can estimate

$$\begin{aligned}
&\sum_{j=1}^{k} \int_0^{t_n} (t_n - s)^{\alpha-1} \left\| s^{\mu-j} \left(s^{j-1} * f^{(k)}(s) \right) \right\|_{L^2(\Omega)} ds \\
&\quad \le kB(\alpha, \mu) t_n^{\alpha+\mu-1} \int_0^{t_n} \left\| f^{(k)}(w) \right\|_{L^2(\Omega)} dw, \ \mu > 0.
\end{aligned}$$

On the other hand, we have

$$\int_0^{t_n} (t_n - s)^{\alpha-1} \left\| s^{\mu} f^{(k)}(s) \right\|_{L^2(\Omega)} ds \le \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu} \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds, \ \mu > -1,$$

and

$$\begin{aligned}
t_n^{\alpha-1} \left\| h^{(k-1)}(0) \right\|_{L^2(\Omega)} &\le c t_n^{\alpha-1} \int_0^{t_n} s^{\mu} \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds \\
&\le c \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu} \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds, \ \mu > -1.
\end{aligned}$$

By the triangle inequality, the desired result is obtained. ∎

THEOREM 5.5. *Let $V(t_n)$ and V^n be the solutions of* (2.4) *and* (2.7)*, respectively. Let $v \in L^2(\Omega)$, $g(t) = t^\mu f(t)$, $\mu > -1$, and $f \in C^{k-1}([0,T]; L^2(\Omega))$ and*

$$\int_0^t \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds < \infty, \quad \int_0^t s^{\frac{\mu-1}{2}} \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds < \infty,$$

and

$$\int_0^t (t-s)^{\alpha-1} s^\mu \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds < \infty.$$

Then the following error estimate holds for any $t_n > 0$:

$$\begin{aligned}
&\|V^n - V(t_n)\|_{L^2(\Omega)} \\
&\le \|J_v\|_{L^2(\Omega)} + \sum_{j=0}^{k-1} \left(c\tau^{\mu+j+m+1} t_n^{\alpha-m-1} + c\tau^k t_n^{\alpha+\mu+j-k} \right) \left\| f^{(j)}(0) \right\|_{L^2(\Omega)} \\
&\quad + c\tau^k \left[t_n^{\alpha+\mu-1} \int_0^{t_n} \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds + t_n^{\alpha+\frac{\mu-1}{2}} \int_0^{t_n} s^{\frac{\mu-1}{2}} \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds \right. \\
&\qquad \left. + \int_0^{t_n} (t_n - s)^{\alpha-1} s^\mu \left\| f^{(k)}(s) \right\|_{L^2(\Omega)} ds \right]
\end{aligned}$$

with $\|J_v\|_{L^2(\Omega)}$ in (3.11).

Proof. Using Theorem 4.4 and Lemma 5.4 and treating the initial data v as in Theorem 3.8, the desired result is obtained. ∎

6. Numerical experiments.

For the sake of brevity, we mainly employ the IDm-BDF6 method in (2.7) for simulating the model (1.1), since similar numerical results can be obtained for the IDm-BDFk with $1 \le m \le k < 6$. We discretize the space direction by the spectral collocation method with the Chebyshev–Gauss–Lobatto points [24]. The discrete L^2-norm ($||\cdot||_{l_2}$) is used to measure the numerical errors at the terminal time, e.g., $t = t_N = 1$. Since the analytic solution is unknown, the convergence rate of the numerical results is computed by

$$\text{Convergence Rate} = \frac{\ln\left(||u^{N/2} - u^N||_{l_2} / ||u^N - u^{2N}||_{l_2}\right)}{\ln 2}.$$

All the numerical experiments are programmed in Julia 1.8.5. One message is that multiple-precision floating-point computation is necessary in order to reduce the round-off errors in evaluating.

Let $T = 1$ and $\Omega = (-1, 1)$. Consider the following two examples:
(a) $v(x) = \sin(x)\sqrt{1-x^2}$ and $g(x,t) = 0$.
(b) $v(x) = \sin(x)\sqrt{1-x^2}$ and $g(x,t) = (1+t^\mu) \circ (e^t + 1) e^x \left(1 + \chi_{(0,1)}(x)\right)$.

Here $G(x,t) = J^m g(x,t) = \frac{t^{m-1}}{\Gamma(m)} * g(x,t)$ in (2.3) is calculated by the JacobiGL algorithm [1, 9], which is generating the nodes and weights of the Gauss–Lobatto integral with the weighting function such as $(1-t)^\mu$ or $(1+t)^\mu$.

Table 6.1 shows that the IDm-BDFk with $k = 6$ recovers high-order convergence, and this is in agreement with Theorem 3.8. In fact, Table 6.1 indicates an optimal error estimate of the Newton–Cotes rule $\mathcal{O}\left(\tau^{\min\{m+1,k\}}\right)$ for odd m and $\mathcal{O}\left(\tau^{\min\{m+2,k\}}\right)$ for even m.

For the subdiffusion model (1.1), it may involve the low regularity or weakly singular source terms [8, 16, 22, 23], e.g.,

$$g(x,t) = t^\mu * f(x,t) \quad \text{or} \quad g(x,t) = t^\mu f(x,t), \quad \mu > -1.$$

In this case, many time-stepping methods, including the correction of high-order BDF schemes [12, 25], are likely to exhibit a severe order reduction (see Table 6.4), since

TABLE 6.1
Case (a): *Convergent order of IDm-BDF*6.

m	$\alpha=0.3$			$\alpha=0.7$		
	$N=200$	$N=400$	$N=800$	$N=200$	$N=400$	$N=800$
1	2.8649e-08	7.1623e-09 1.9999	1.7905e-09 2.0000	5.8503e-08	1.4626e-08 1.9999	3.6565e-09 2.0000
2	3.4067e-13	2.0551e-14 4.0511	1.2734e-15 4.0124	1.0704e-12	6.3277e-14 4.0804	3.9010e-15 4.0197
3	8.5708e-14	6.4330e-15 3.7358	4.1808e-16 3.9436	2.2754e-13	1.9161e-14 3.5699	1.2708e-15 3.9143
4	2.9657e-14	4.4445e-16 6.0602	6.8021e-18 6.0298	1.3125e-13	1.9603e-15 6.0651	2.9951e-17 6.0323
5	3.6694e-14	5.4991e-16 6.0602	8.4162e-18 6.0298	1.5877e-13	2.3712e-15 6.0652	3.6228e-17 6.0323
6	4.3721e-14	6.5521e-16 6.0602	1.0027e-17 6.0298	1.8626e-13	2.7815e-15 6.0652	4.2496e-17 6.0324

TABLE 6.2
Case (b) *with convolution: Convergent order of IDm-BDF*6.

m	$\alpha=0.3,\mu=-0.4$			$\alpha=0.7,\mu=0.3$		
	$N=200$	$N=400$	$N=800$	$N=200$	$N=400$	$N=800$
1	2.8489e-08	7.1310e-09 1.9982	1.7848e-09 1.9982	5.8505e-08	1.4626e-08 2.0000	3.6565e-09 2.0000
2	5.2663e-12	4.2479e-13 3.6319	3.4655e-14 3.6156	1.3146e-12	8.0904e-14 4.0222	5.0214e-15 4.0100
3	1.4691e-13	7.0242e-15 4.3865	4.2499e-16 4.0468	2.4212e-13	1.8753e-14 3.6905	1.2629e-15 3.8923
4	1.2361e-13	1.8343e-15 6.0743	2.7925e-17 6.0375	2.6971e-13	4.0850e-15 6.0449	6.2856e-17 6.0221
5	1.5665e-13	2.3252e-15 6.0187	3.5406e-17 6.0093	3.3626e-13	5.0941e-15 6.0446	7.8391e-17 6.0220
6	1.8965e-13	2.8153e-15 6.0739	4.2870e-17 6.0372	4.0290e-13	6.1045e-15 6.0444	9.3946e-17 6.0219

TABLE 6.3
Case (b) *with product: Convergent order of IDm-BDF*6.

m	$\alpha=0.3,\mu=-0.4$			$\alpha=0.7,\mu=0.3$		
	$N=200$	$N=400$	$N=800$	$N=200$	$N=400$	$N=800$
1	5.6978e-06	1.8615e-06 1.6138	6.0971e-07 1.61033	7.0952e-07	1.7474e-07 2.0216	4.3146e-08 2.0179
2	4.7855e-09	7.9295e-10 2.5933	1.3108e-10 2.59671	6.1995e-11	5.8815e-12 3.3979	5.7317e-13 3.35914
3	1.7095e-11	1.3407e-12 3.6725	1.0870e-13 3.62449	2.5149e-12	1.7869e-13 3.8149	1.1382e-14 3.97267
4	9.9716e-13	1.4047e-14 6.1494	1.7852e-16 6.2981	7.2236e-13	1.0853e-14 6.0565	1.6622e-16 6.02881
5	1.3010e-12	1.9509e-14 6.0593	2.9866e-16 6.02948	9.2805e-13	1.3945e-14 6.0562	2.1371e-16 6.02803
6	1.5714e-12	2.3564e-14 6.0592	3.6077e-16 6.02938	1.1330e-12	1.7023e-14 6.0565	2.6085e-16 6.02815

it is required that the function $g \in C^{k-1}([0,T];L^2(\Omega))$. In fact, for the low regularity source term $g(x,t)=t^{\mu}$, $\mu>0$, the correction of the BDF2 (Corr-BDF2) scheme converges with the order $\mathcal{O}(\tau^{1+\mu})$; see Lemma 3.2 in [31]. To fill in this gap, the desired kth-order convergence rate can be recovered by the IDm-BDFk method, which is characterized by Theorems 5.2 and 5.5; see Tables 6.2 and 6.3, respectively.

Table 6.4
Case (b) *with product: Comparison of several methods.*

Scheme	$\alpha = 0.3, \mu = -0.4$			$\alpha = 0.7, \mu = 0.3$		
	$N = 200$	$N = 400$	$N = 800$	$N = 200$	$N = 400$	$N = 800$
BDF2	1.9996e-03	1.2957e-03 0.6259	8.4321e-04 0.6198	3.5185e-04	1.7321e-04 1.0224	8.5275e-05 1.0223
Corr-BDF2	NaN	NaN —	NaN —	2.6235e-05	1.1807e-05 1.1517	5.0842e-06 1.2156
ID2-BDF2	4.7799e-05	1.1962e-05 1.9985	2.9920e-06 1.9992	4.6997e-05	1.1794e-05 1.9945	2.9541e-06 1.9972
BDF4	2.0020e-03	1.2964e-03 0.6269	8.4336e-04 0.6202	3.5870e-04	1.7493e-04 1.0360	8.5705e-05 1.0292
Corr-BDF4	NaN	NaN —	NaN —	NaN	NaN —	NaN —
ID4-BDF4	1.8228e-09	1.1510e-10 3.9850	7.2311e-12 3.9926	2.7000e-09	1.6848e-10 4.0023	1.0522e-11 4.0011

7. Conclusions.

The subdiffusion models can involve the singular source term, which exhibits a severe order reduction by many time-stepping methods. In this work we first derive an optimal error estimate of the kth-order Newton–Cotes rule $\mathcal{O}\left(\tau^{\min\{m+1,k\}}\right)$ for odd m and $\mathcal{O}\left(\tau^{\min\{m+2,k\}}\right)$ for even m, $1 \leq m \leq k \leq 6$, under the mild regularity of the source function. Then the desired kth-order convergence rate is well developed by the smoothing method under the certainly singular source terms. It is interesting to design the numerical algorithms for the nonlinear fractional models.

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