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MODIFIED BDF2 SCHEMES FOR SUBDIFFUSION MODELS WITH A SINGULAR SOURCE TERM

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Abstract. The aim of this paper is to study the time stepping scheme for approximately solving the subdiffusion equation with a weakly singular source term. In this case, many popular time stepping schemes, including the correction of high-order BDF methods, may lose their high-order accuracy. To fill in this gap, in this paper, we develop a novel time stepping scheme, where the source term is regularized by using a k-fold integral-derivative and the equation is discretized by using a modified BDF2 convolution quadrature. We prove that the proposed time stepping scheme is second-order, even if the source term is nonsmooth in time and incompatible with the initial data. Numerical results are presented to support the theoretical results.

Key words. subdiffusion, modified BDF2 schemes, singular source term, error estimate

AMS subject classifications.

1. Introduction.

For anomalous, non-Brownian diffusion, a mean squared displacement often follows the following power-law

$$\langle x^2(t)\rangle \simeq K_\alpha t^\alpha.$$

Prominent examples for subdiffusion include the classical charge carrier transport in amorphous semiconductors, tracer diffusion in subsurface aquifers, porous systems, dynamics of a bead in a polymeric network, or the motion of passive tracers in living biological cells [18, 19]. Subdiffusion of this type is characterised by a long-tailed waiting time probability density function $\psi(t) \simeq t^{-1-\alpha}$, corresponding to the time-fractional diffusion equation with and without an external force field [19, Eq. (88)]

$$(\spadesuit) \qquad \partial_t u(x,t) - \partial_t^{1-\alpha} A u(x,t) = f(x,t), \quad 0<\alpha<1.$$

Here f is a given source function, and the operator $A = \Delta$ denotes Laplacian on a polyhedral domain $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$ with a homogenous Dirichlet boundary condition. The fractional derivative is taken in the Riemann-Liouville sense, that is, $\partial_t^{1-\alpha} f = \partial_t J^\alpha f$ with the fractional integration operator

$$J^\alpha f(t) = \frac{1}{\Gamma(\alpha)}\int_0^t (t-\tau)^{\alpha-1} f(\tau)d\tau = \frac{1}{\Gamma(\alpha)} t^{\alpha-1} * f(t),$$

and $*$ denotes the Laplace convolution: $(f * g)(t) = \int_0^t f(t-\tau)g(\tau)d\tau$.

Since the Riemann-Liouvile fractional derivative and the Caputo fractional derivative can be written in the form [22, p. 76]

$$\partial_t^\alpha u(x,t) = {}^C D_t^\alpha u(x,t) + \frac{1}{\Gamma(1-\alpha)} t^{-\alpha} u(x,0),$$

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which implies that the equivalent form of (♠) can be rewritten as

$$(\heartsuit) \qquad \partial_t u(x,t) - {}^C D_t^{1-\alpha} Au(x,t) = f(x,t) + \frac{Au(x,0)}{\Gamma(\alpha)} t^{-(1-\alpha)}, \quad 0 < \alpha < 1$$

with the Caputo fractional derivative

$${}^C D_t^{\alpha} u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u'(s) ds, \quad 0 < t \le T.$$

Applying the fractional integration operator $J^{1-\alpha}$ to both sides of (♠), we obtain the equivalent form of (♠) as, see [17, Eq. (1.6)] or [26, Eq. (2.3)], namely,

$$(\clubsuit) \quad {}^C D_t^{\alpha} u(x,t) - Au(x,t) = \frac{1}{\Gamma(1-\alpha)} t^{-\alpha} * f(x,t) - \frac{J^{\alpha} Au(x,t)|_{t=0}}{\Gamma(1-\alpha)} t^{-\alpha}, \ 0 < \alpha < 1.$$

As another example, the fractal mobile/immobile models for solute transport associate with power law decay PDF describing random waiting times in the immobile zone, leads to the following models [24, Eq. (15)]

$$(\diamondsuit) \qquad \partial_t u(x,t) + {}^C D_t^{\alpha} u(x,t) - Au(x,t) = -\frac{1}{\Gamma(1-\alpha)} t^{-\alpha} u(x,0), \ 0 < \alpha < 1.$$

Note that the right hand side in aforementioned PDE models (♠)-(♢) might be nonsmooth in the time variable. In this paper, we consider the subdiffusion model with weakly singular source term:

$$(1.1) \qquad {}^C D_t^{\alpha} u(x,t) - Au(x,t) = g(x,t) := t^{\mu} \circ f(x,t)$$

with the initial condition $u(x,0) = u_0(x) := v$, and the homogeneous Dirichlet boundary conditions. The symbol $\circ$ can be either the convolution $*$ or the product, and μ is a parameter such that

$$\mu > -1 \ \text{ if } \circ \text{ denotes convolution, } \ \text{ and } \ \mu \ge -\alpha \ \text{ if } \circ \text{ denotes product.}$$

The well-posedness could be proved using the separation of variables and Mittag–Leffler functions, see e.g. [23, Eq. (2.11)].

Note that many existing time stepping schemes may lose their high-order accuracy when the source term is nonsmooth in the time variable. As an example, it was reported in [10, Section 4.1] that the convolution quadrature generated by k step BDF method (with initial correction) converges with order $O(\tau^{1+\mu})$, provided that the source term behaves like t^{μ}, $\mu > 0$, see Lemma 3.2 in [31], also see Table 6.1. The aim of this paper is to fill in this gap.

It is well-known that the smoothness of all the data of (1.1) (e.g., $f = 0$) do not imply the smoothness of the solution u which has an initial layer at $t \to 0^+$ (i.e., unbounded near $t = 0$) [22, 23, 28]. There are already two predominant discretization techniques in time direction to restore the desired convergence rate for subdiffusion under appropriate regularity source function. The first type is that the nonuniform time meshes/graded meshes are employed to compensate/capture the singularity of the continuous solution near $t = 0$ under the appropriate regularity source function and initial data, see [3, 11, 13, 16, 20, 21, 28]. See also spectral method with specially designed basis functions [4, 8, 33]. The second type is that, based on correction of high-order BDFk or L_k approximation, the desired high-order convergence rates can be restored even for nonsmooth initial data. For fractional ODEs, one idea is to use starting quadrature weights to correct the fractional integrals [14] (or fractional substantial calculus [1])

$$J^\alpha g(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} g(\tau) d\tau \quad \text{with} \quad g(t) = t^\mu f(t), \quad \mu > -1,$$

where the algorithms rely on expanding the solution into power series of t. For fractional PDEs, a common practice is to split the source term into

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

Then approximating $g(0)$ by $\partial_\tau J^1 g(0)$ may to a modified BDF2 scheme with correction in the first step [5]. The correction of high-order BDFk or L_k convolution quadrature are well developed in [10, 27, 32] when the source term sufficiently smooth in the time variable. Performing the integral on both sides for (1.1), e.g, approximate $u(t)$ by $\partial_\tau J^1 u(t)$, a second-order time-stepping schemes are given in [34], where the singular source function is $g(x,t) = t^\mu f(x)$ with a spatially dependent function f. How to deal with a more general source term, which might be nonsmooth in the time variable, is still unavailable in the literature.

In this paper, we develop a novel second-order time stepping scheme (IDk-BDF2) for solving the subdiffusion (1.1) with a weakly singular source term, where the low regularly source term is regularized by using a k-fold integral-derivative (IDk) and the equation is discretized by using a modified BDF2 convolution quadrature. We prove that the proposed time stepping scheme is second-order, even if the source term is nonsmooth in time and incompatible with the initial data. Numerical results are presented to support the theoretical results.

The paper is organized as follows. In Section 2, we introduce the development of the IDk-BDF2 scheme for model (1.1). In Section 3 and 4, based on operational calculus, the detailed convergence analysis of IDk-BDF2 are provided, respectively, for general source function $f(x,t)$ and certain form $t^\mu f(x)$. Then the desired results with the low regularity source term $t^\mu \circ f(x,t)$ are obtained in Section 5. To show the effectiveness of the presented schemes, the results of numerical experiments are reported in Section 6. Finally, we conclude the paper with some remarks in the last section.

2. IDk-BDF2 Method. In this section, we first provide IDk-BDF2 method for solving subdiffusion (1.1) if the source term $g(x,t)$ possess the mild regularity. Let $V(t) = u(t) - v$ with $V(0) = 0$. Then the model (1.1) can be rewritten as

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

From [15] and [29], we know that the operator A satisfies the following resolvent estimate

$$\left\|(z-A)^{-1}\right\| \leq c_\phi |z|^{-1} \quad \forall z \in \Sigma_\phi$$

for all $\phi \in (\pi/2, \pi)$, where $\Sigma_\theta := \{z \in \mathbb{C}\backslash\{0\} : |\arg z| < \theta\}$ is a sector of the complex plane $\mathbb{C}$. Hence, $z^\alpha \in \Sigma_{\theta'}$ with $\theta' = \alpha\theta < \theta < \pi$ for all $z \in \Sigma_\theta$. Then, there exists a positive constant c such that

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

2.1. Discretization schemes. Let $G(t) = J^1 g(t)$ and $\mathcal{G}(t) = J^2 g(t)$. By first fundamental theorem of calculus, we may rewrite (2.1) as

$$\text{ID1 Method}: \ \partial_t^\alpha V(t) - AV(t) = \partial_t (tAv + G(t)), \quad 0 < t \le T, \tag{2.3}$$

$$\text{ID2 Method}: \ \partial_t^\alpha V(t) - AV(t) = \partial_t^2 \left(\frac{t^2}{2} Av + \mathcal{G}(t) \right), \quad 0 < t \le T. \tag{2.4}$$

Let $t_n = n\tau, n = 0, 1, \ldots, N$, be a uniform partition of the time interval $[0, T]$ with the step size $\tau = \frac{T}{N}$, and let u^n denote the approximation of $u(t)$ and $g^n = g(t_n)$. The convolution quadrature generated by BDF2 approximates the Riemann-Liouville fractional derivative $\partial_t^\alpha \varphi(t_n)$ by

$$\partial_\tau^\alpha \varphi^n := \frac{1}{\tau^\alpha} \sum_{j=0}^{n} \omega_j \varphi^{n-j} \tag{2.5}$$

with $\varphi^n = \varphi(t_n)$. Here the weights ω_j are the coefficients in the series expansion

$$\delta_\tau^\alpha(\xi) = \frac{1}{\tau^\alpha} \sum_{j=0}^{\infty} \omega_j \xi^j \quad \text{with} \quad \delta_\tau(\xi) := \frac{1}{\tau} \left(\frac{3}{2} - 2\xi + \frac{1}{2}\xi^2 \right). \tag{2.6}$$

Then IDk-BDF2 method for (2.3) and (2.4) are, respectively, designed by

$$\text{ID1} - \text{BDF2 Method}: \quad \partial_\tau^\alpha V^n - AV^n = \partial_\tau (t_n Av + G^n). \tag{2.7}$$

$$\text{ID2} - \text{BDF2 Method}: \quad \partial_\tau^\alpha V^n - AV^n = \partial_\tau^2 \left(\frac{t_n^2}{2} Av + \mathcal{G}^n \right). \tag{2.8}$$

REMARK 2.1. *In the time semidiscrete approximation* (2.7) *and* (2.8)*, we require* $v \in \mathcal{D}(A)$*, i.e., the initial data* v *is reasonably smooth. However one can use the schemes* (2.7) *and* (2.8) *to prove the error estimates with the nonsmooth data* $v \in L^2(\Omega)$*, see Theorems 5.4 and 5.6. Here, we mainly focus on the time semidiscrete approximation* (2.7) *and* (2.8)*, since the spatial discretization is well understood. For example, we choose* $v_h = R_h v$ *if* $v \in \mathcal{D}(A)$ *and* $v_h = P_h v$ *if* $v \in L^2(\Omega)$ *following [29, 30].*

2.2. Solution representation for (2.3) **and** (2.4)**.** Taking the Laplace transform in both sides of (2.3), it leads to

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

By the inverse Laplace transform, there exists [10]

$$V(t) = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}} e^{zt} (z^\alpha - A)^{-1} \left(z^{-1} Av + z\widehat{G}(z) \right) dz \tag{2.9}$$

with

$$\Gamma_{\theta,\kappa} = \{ z \in \mathbb{C} : |z| = \kappa, |\arg z| \le \theta \} \cup \{ z \in \mathbb{C} : z = re^{\pm i\theta}, r \ge \kappa \} \tag{2.10}$$

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

Similarly, applying the Laplace transform in both sides of (2.4), it yields

$$\widehat{V}(z) = (z^\alpha - A)^{-1} \left(z^{-1} A v + z^2 \widehat{\mathcal{G}}(z) \right).$$

By the inverse Laplace transform, we obtain

$$V(t) = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}} e^{zt} (z^\alpha - A)^{-1} \left(z^{-1} A v + z^2 \widehat{\mathcal{G}}(z) \right) dz. \tag{2.11}$$

2.3. Discrete solution representation for (2.7) **and** (2.8)**.** Given a sequence $(\kappa_n)_0^\infty$ and take $\widetilde{\kappa}(\zeta) = \sum_{n=0}^\infty \kappa_n \zeta^n$ to be its generating power series.

LEMMA 2.1. *Let δ_τ be given in* (2.6) *and $\gamma_1(\xi) = \frac{\xi}{(1-\xi)^2}$, $G(t) = J^1 g(t)$. Then the discrete solution of* (2.7) *is represented by*

$$V^n = \frac{1}{2\pi i} \int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n} (\delta^\alpha_\tau(e^{-z\tau}) - A)^{-1} \delta_\tau(e^{-z\tau}) \tau \left(\gamma_1(e^{-z\tau}) \tau A v + \widetilde{G}(e^{-z\tau}) \right) dz$$

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

Proof. Multiplying the (2.7) by ξ^n and summing over n with $V^0 = 0$, we obtain

$$\sum_{n=1}^\infty \partial^\alpha_\tau V^n \xi^n - \sum_{n=1}^\infty A V^n \xi^n = \sum_{n=1}^\infty \partial_\tau (t_n A v + G^n) \xi^n.$$

From (2.5) and (2.6), we have

$$\begin{aligned} \sum_{n=1}^\infty \partial^\alpha_\tau V^n \xi^n &= \sum_{n=1}^\infty \frac{1}{\tau^\alpha} \sum_{j=0}^n \omega_j V^{n-j} \xi^n = \sum_{n=0}^\infty \frac{1}{\tau^\alpha} \sum_{j=0}^n \omega_j V^{n-j} \xi^n = \sum_{j=0}^\infty \frac{1}{\tau^\alpha} \sum_{n=j}^\infty \omega_j V^{n-j} \xi^n \\ &= \sum_{j=0}^\infty \frac{1}{\tau^\alpha} \sum_{n=0}^\infty \omega_j V^n \xi^{n+j} = \frac{1}{\tau^\alpha} \sum_{j=0}^\infty \omega_j \xi^j \sum_{n=0}^\infty V^n \xi^n = \delta^\alpha_\tau(\xi) \widetilde{V}(\xi). \end{aligned}$$

Similarly, one has

$$\sum_{n=1}^\infty \partial_\tau t_n A v \xi^n = \delta_\tau(\xi) \gamma_1(\xi) \tau A v, \quad \sum_{n=1}^\infty \partial_\tau G^n \xi^n = \delta_\tau(\xi) \widetilde{G}(\xi)$$

with $\gamma_1(\xi) = \frac{\xi}{(1-\xi)^2}$. It leads to

$$\widetilde{V}(\xi) = (\delta^\alpha_\tau(\xi) - A)^{-1} \delta_\tau(\xi) \left(\gamma_1(\xi) \tau A v + \widetilde{G}(\xi) \right). \tag{2.12}$$

According to Cauchy's integral formula, and the change of variables $\xi = e^{-z\tau}$, and Cauchy's theorem, one has [10]

$$V^n = \frac{\tau}{2\pi i} \int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n} \left(\delta^\alpha_\tau(e^{-z\tau}) - A \right)^{-1} \delta_\tau(e^{-z\tau}) \left(\gamma_1(e^{-z\tau}) \tau A v + \widetilde{G}(e^{-z\tau}) \right) dz \tag{2.13}$$

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

LEMMA 2.2. *Let δ_τ be given in* (2.6) *and $\gamma_2(\xi) = \frac{\xi+\xi^2}{(1-\xi)^3}$, $\mathcal{G}(t) = J^2 g(t)$. Then the discrete solution of* (2.8) *is represented by*

$$V^n = \frac{\tau}{2\pi i} \int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n} \left(\delta^\alpha_\tau(e^{-z\tau}) - A \right)^{-1} \delta^2_\tau(e^{-z\tau}) \left(\frac{\gamma_2(e^{-z\tau})}{2} \tau^2 A v + \widetilde{\mathcal{G}}(e^{-z\tau}) \right) dz$$

with $\Gamma^{\tau}_{\theta,\kappa} = \{z \in \Gamma_{\theta,\kappa} : |\Im z| \le \pi/\tau\}$.

Proof. Multiplying the (2.8) by ξ^n and summing over n with $V^0 = 0$, we obtain

$$\sum_{n=1}^{\infty} \partial_\tau^\alpha V^n \xi^n - \sum_{n=1}^{\infty} AV^n \xi^n = \sum_{n=1}^{\infty} \partial_\tau^2 \left(\frac{t_n^2}{2} Av + \mathcal{G}^n \right) \xi^n.$$

The similar arguments can be performed as Lemma 2.1, it yields

$$\sum_{n=1}^{\infty} \partial_\tau^\alpha V^n \xi^n = \delta_\tau^\alpha(\xi) \widetilde{V}(\xi), \quad \sum_{n=1}^{\infty} \partial_\tau^2 t_n^2 Av \xi^n = \delta_\tau^2(\xi)\gamma_2(\xi)\tau^2 Av,$$
$$\sum_{n=1}^{\infty} \partial_\tau^2 \mathcal{G}^n \xi^n = \delta_\tau^2(\xi)\widetilde{\mathcal{G}}(\xi), \quad \gamma_2(\xi) = \frac{\xi + \xi^2}{(1-\xi)^3},$$

and

$$\widetilde{V}(\xi) = \left(\delta_\tau^\alpha(\xi) - A\right)^{-1} \delta_\tau^2(\xi) \left(\frac{\gamma_2(\xi)}{2} \tau^2 Av + \widetilde{\mathcal{G}}(\xi) \right). \tag{2.14}$$

Using Cauchy's integral formula, and the change of variables $\xi = e^{-z\tau}$, and Cauchy's theorem, one has

$$V^n = \frac{\tau}{2\pi i} \int_{\Gamma^{\tau}_{\theta,\kappa}} e^{zt_n} \left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} \delta_\tau^2(e^{-z\tau}) \left(\frac{\gamma_2(\xi)}{2} \tau^2 Av + \widetilde{\mathcal{G}}(e^{-z\tau}) \right) dz \tag{2.15}$$

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 $g(x,t)$.

In this section, we provide the detailed convergence analysis of ID1-BDF2 in (2.7) approximation for the subdiffusion (2.3), and ID2-BDF2 can be similarly augmented.

3.1. A few technical lemmas.

First, we give some lemmas that will be used.

LEMMA 3.1. *[10] Let* $\delta_\tau(\xi)$ *be given in* (2.6). *Then there exist the positive constants* c_1, c_2, c *and* $\theta \in (\pi/2, \theta_\varepsilon)$ *with* $\theta_\varepsilon \in (\pi/2, \pi)$, $\forall \varepsilon > 0$ *such that*

$$c_1|z| \le |\delta_\tau(e^{-z\tau})| \le c_2|z|, \quad |\delta_\tau(e^{-z\tau}) - z| \le c\tau^2|z|^3,$$
$$|\delta_\tau^\alpha(e^{-z\tau}) - z^\alpha| \le c\tau^2|z|^{2+\alpha}, \ \delta_\tau(e^{-z\tau}) \in \Sigma_{\pi/2+\varepsilon} \quad \forall z \in \Gamma^{\tau}_{\theta,\kappa}.$$

LEMMA 3.2. *Let* $\delta_\tau(\xi)$ *be given in* (2.6) *and* $\gamma_l(\xi) = \sum_{n=1}^{\infty} n^l \xi^n = \left(\xi \frac{d}{d\xi}\right)^l \frac{1}{1-\xi}$ *with* $l = 0, 1, 2$. *Then there exist a positive constants* c *such that*

$$\left| \frac{\gamma_l(e^{-z\tau})}{l!} \tau^{l+1} - z^{-l-1} \right| \le c\tau^{l+1}, \quad \forall z \in \Gamma^{\tau}_{\theta,\kappa},$$

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

Proof. The arguments can be performed in [27] for $l = 1, 2$. For $l = 0$, using

$$\frac{1}{1 - e^{-z\tau}} \tau - z^{-1} = \frac{z - (1 - e^{-z\tau})\,\tau^{-1}}{(1 - e^{-z\tau})\,\tau^{-1} z},$$

and Lemma 3.1, it yields $|1 - e^{-z\tau}| \ge c_1|z|\tau$ and

$$\left|(1 - e^{-z\tau})\tau^{-1} z\right| \ge c|z|^2 \quad \forall z \in \Gamma^{\tau}_{\theta,\kappa}. \tag{3.1}$$

Since

$$\left|z-\left(1-e^{-z\tau}\right)\tau^{-1}\right| = \left|z-\left(1-\sum_{j=0}^{\infty}\frac{(-z\tau)^j}{j!}\right)\tau^{-1}\right| = \left|z-\left(-\sum_{j=1}^{\infty}\frac{(-z\tau)^j}{j!}\right)\tau^{-1}\right|$$
$$= \left|z-z\sum_{j=0}^{\infty}\frac{(-z\tau)^j}{(j+1)!}\right| = \left|\tau z^2\sum_{j=0}^{\infty}\frac{(-z\tau)^j}{(j+2)!}\right| \le c\tau\left|z\right|^2.$$

Thus we have

$$\left|\frac{1}{1-e^{-z\tau}}\tau - z^{-1}\right| \le c\tau.$$

The proof is completed. □

LEMMA 3.3. *Let $\delta_\tau(\xi)$ be given in (2.6) and $\gamma_l(\xi)=\sum_{n=1}^{\infty}n^l\xi^n = \left(\xi\frac{d}{d\xi}\right)^l\frac{1}{1-\xi}$ with $l=0,1,2$. Then there exist a positive constants c such that*

$$\left|\delta_\tau(e^{-z\tau})\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-z^{-l}\right| \le c\tau^{l+1}\left|z\right| + c\tau^2|z|^{2-l}, \quad \forall z\in\Gamma_{\theta,\kappa}^{\tau}, \tag{3.2}$$

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

Proof. Let

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

with

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

According to Lemma 3.1 and 3.2, we have

$$|J_1| = \left|\delta_\tau(e^{-z\tau})\left(\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-z^{-l-1}\right)\right| \le c_2\left|z\right|c\tau^{l+1} \le c\tau^{l+1}\left|z\right|$$

and

$$|J_2| = \left|\left(\delta_\tau(e^{-z\tau})-z\right)z^{-l-1}\right| \le c\tau^2|z|^{2-l}.$$

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

LEMMA 3.4. *Let δ_τ^α be given by (2.6) and $\gamma_l(\xi)=\sum_{n=1}^{\infty}n^l\xi^n=\left(\xi\frac{d}{d\xi}\right)^l\frac{1}{1-\xi}$ with $l=0,1,2$. Then there exist a positive constants c such that*

$$\left\|\left(\delta_\tau^\alpha(e^{-z\tau})-A\right)^{-1}\delta_\tau(e^{-z\tau})\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-(z^\alpha-A)^{-1}z^{-l}\right\|$$
$$\le c\tau^{l+1}\left|z\right|^{1-\alpha}+c\tau^2|z|^{2-l-\alpha}.$$

Proof. Let

$$\left(\delta_\tau^\alpha(e^{-z\tau})-A\right)^{-1}\delta_\tau(e^{-z\tau})\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1}-(z^\alpha-A)^{-1}z^{-l}=I+II$$

with

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

The resolvent estimate (2.2) and Lemma 3.1 imply directly

$$\|\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\| \le c|z|^{-\alpha}. \tag{3.3}$$

From (3.3) and Lemma 3.3, we obtain

$$\|I\| \le c\tau^{l+1}|z|^{1-\alpha} + c\tau^2|z|^{2-l-\alpha}.$$

Using Lemma 3.1, (3.3) and the identity

$$\begin{aligned}&\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} - (z^\alpha - A)^{-1}\\ &\quad = \left(z^\alpha - \delta_\tau^\alpha(e^{-z\tau})\right)\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}(z^\alpha - A)^{-1},\end{aligned} \tag{3.4}$$

we estimate II as following

$$\|II\| \le c\tau^2|z|^{2+\alpha}c|z|^{-\alpha}c|z|^{-\alpha}|z|^{-l} \le c\tau^2|z|^{2-l-\alpha}.$$

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

LEMMA 3.5. *Let δ_τ^α be given by (2.6) and $\gamma_1(\xi) = \sum_{n=1}^\infty n\xi^n = \left(\xi\frac{d}{d\xi}\right)\frac{1}{1-\xi} = \frac{\xi}{(1-\xi)^2}$. Then there exist a positive constants c such that*

$$\left\|\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\delta_\tau(e^{-z\tau})\gamma_1(e^{-z\tau})\tau^2 A - (z^\alpha - A)^{-1}z^{-1}A\right\| \le c\tau^2|z|.$$

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

$$\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\delta_\tau(e^{-z\tau})A = -\delta_\tau(e^{-z\tau}) + \left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\delta_\tau^\alpha(e^{-z\tau})\delta_\tau(e^{-z\tau})A,$$

we get

$$\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\delta_\tau(e^{-z\tau})\gamma_1(e^{-z\tau})\tau^2 A - (z^\alpha - A)^{-1}z^{-1}A = J_1 + J_2 + J_3 + J_4$$

with

$$J_1 = \left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\delta_\tau^\alpha(e^{-z\tau})\left(\delta_\tau(e^{-z\tau})\gamma_1(e^{-z\tau})\tau^{l+1} - z^{-1}\right),$$
$$J_2 = \left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\left(\delta_\tau^\alpha(e^{-z\tau}) - z^\alpha\right)z^{-1},$$
$$J_3 = \left(\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} - (z^\alpha - A)^{-1}\right)z^{\alpha-1}, \quad J_4 = z^{-1} - \delta_\tau(e^{-z\tau})\gamma_1(e^{-z\tau})\tau^2.$$

According to (3.3) and Lemmas 3.1, 3.3 with $l = 1$, we estimate J_1, J_2 and J_4 as following

$$\|J_1\| \le c|z|^{-\alpha}|z|^\alpha\tau^2|z| \le c\tau^2|z|,$$
$$\|J_2\| \le c|z|^{-\alpha}\tau^2|z|^{2+\alpha}|z|^{-1} \le c\tau^2|z|, \quad \|J_4\| \le c\tau^2|z|.$$

From Lemma 3.1, (3.3) and the identity (3.4), we estimate J_3 as following

$$\|J_3\| \le c\tau^2|z|^{2+\alpha}|z|^{-\alpha}|z|^{-\alpha}|z|^{\alpha-1} \le c\tau^2|z|.$$

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

3.2. Error analysis for general source function $g(x,t)$. From $G(t) = J^1 g(t)$, the Taylor expansion of source function with the remainder term in integral form:

$$\begin{aligned} 1 * g(t) = G(t) &= G(0) + tG'(0) + \frac{t^2}{2}G''(0) + \frac{t^2}{2} * G'''(t) \\ &= J^1 g(0) + tg(0) + \frac{t^2}{2}g'(0) + \frac{t^2}{2} * g''(t). \end{aligned}$$

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

LEMMA 3.6. *Let $V(t_n)$ and V^n be the solutions of* (2.3) *and* (2.7)*, respectively. Let $v = 0$ and $G(t) := \frac{t^l}{l!} g^{(l-1)}(0)$ with $l = 0, 1, 2$. Then*

$$\|V(t_n) - V^n\| \leq \left(c\tau^{l+1} t_n^{\alpha-2} + c\tau^2 t_n^{\alpha+l-3}\right) \left\|g^{(l-1)}(0)\right\|. \tag{3.5}$$

Proof. Using (2.9) and (2.13), there exist

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

and

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

where $\theta \in (\pi/2, \pi)$ is sufficiently close to $\pi/2$, and $\gamma_l(\xi) = \sum_{n=1}^\infty n^l \xi^n$. Let

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

with

$$J_1 = \frac{1}{2\pi i} \int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n} \left[\frac{(z^\alpha - A)^{-1}}{z^l} - \left(\delta^\alpha_\tau(e^{-z\tau}) - A\right)^{-1} \delta_\tau(e^{-z\tau}) \frac{\gamma_l(e^{-z\tau})}{l!} \tau^{l+1}\right] g^{(l-1)}(0) dz,$$

and

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

According to the triangle inequality, (2.2) and Lemma 3.4, one has

$$\begin{aligned} \|J_1\| \leq{}& c \int_\kappa^{\frac{\pi}{\tau \sin\theta}} e^{rt_n \cos\theta} \left(\tau^{l+1} r^{1-\alpha} + \tau^2 r^{2-l-\alpha}\right) dr \left\|g^{(l-1)}(0)\right\| \\ &+ c \int_{-\theta}^{\theta} e^{\kappa t_n \cos\psi} \left(\tau^{l+1} \kappa^{2-\alpha} + \tau^2 \kappa^{3-l-\alpha}\right) d\psi \left\|g^{(l-1)}(0)\right\| \\ \leq{}& \left(c\tau^{l+1} t_n^{\alpha-2} + c\tau^2 t_n^{\alpha+l-3}\right) \left\|g^{(l-1)}(0)\right\|, \end{aligned}$$

for the last inequality, we use

$$\begin{aligned} &\int_\kappa^{\frac{\pi}{\tau\sin\theta}} e^{rt_n\cos\theta} r^{2-l-\alpha} dr = t_n^{\alpha+l-3} \int_{t_n\kappa}^{\frac{t_n\pi}{\tau\sin\theta}} e^{s\cos\theta} s^{2-l-\alpha} ds \leq ct_n^{\alpha+l-3}, \\ &\int_{-\theta}^{\theta} e^{\kappa t_n\cos\psi} \kappa^{3-l-\alpha} d\psi = t_n^{\alpha+l-3} \int_{-\theta}^{\theta} e^{\kappa t_n \cos\psi} \left(\kappa t_n\right)^{3-l-\alpha} d\psi \leq ct_n^{\alpha+l-3}. \end{aligned} \tag{3.6}$$

From (2.2), it yields

$$\begin{aligned}\|J_2\| &\le c\left\|g^{(l-1)}(0)\right\|\int_{\frac{\pi}{\tau\sin\theta}}^{\infty} e^{rt_n\cos\theta} r^{-l-\alpha}dr\\ &\le c\tau^2\left\|g^{(l-1)}(0)\right\|\int_{\frac{\pi}{\tau\sin\theta}}^{\infty} e^{rt_n\cos\theta} r^{2-l-\alpha}dr \le c\tau^2 t_n^{\alpha+l-3}\left\|g^{(l-1)}(0)\right\|.\end{aligned}$$

Here we using $1 \le (\frac{\sin\theta}{\pi})^2\tau^2 r^2$ with $r \ge \frac{\pi}{\tau\sin\theta}$. The proof is completed. □

LEMMA 3.7. *Let $V(t_n)$ and V^n be the solutions of (2.3) and (2.7), respectively. Let $v = 0$, $G(t) := \frac{t^2}{2} * g''(t)$ and $\int_0^t (t-s)^{\alpha-1}\|g''(s)\|ds < \infty$. Then*

$$\|V(t_n) - V^n\| \le c\tau^2\int_0^{t_n}(t_n - s)^{\alpha-1}\|g''(s)\|\,ds.$$

Proof. By (2.9), we obtain

$$\begin{aligned}V(t_n) &= \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{zt_n}(z^\alpha - A)^{-1} z\widehat{G}(z)dz = (\mathscr{E}(t) * G(t))(t_n)\\ &= \left(\mathscr{E}(t) * \left(\frac{t^2}{2} * g''(t)\right)\right)(t_n) = \left(\left(\mathscr{E}(t) * \frac{t^2}{2}\right) * g''(t)\right)(t_n)\end{aligned} \tag{3.7}$$

with

$$\mathscr{E}(t) = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{zt}(z^\alpha - A)^{-1} z dz. \tag{3.8}$$

From (2.12), it yields

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

with

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

Here $\sum_{n=0}^{\infty}\mathscr{E}_\tau^n\xi^n = \widetilde{\mathscr{E}_\tau}(\xi) = (\delta_\tau^\alpha(\xi) - A)^{-1}\delta_\tau(\xi)$. From the Cauchy's integral formula and the change of variables $\xi = e^{-z\tau}$, we obtain the representation of the $\mathscr{E}_\tau^n$ as following

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

where $\theta \in (\pi/2, \pi)$ is sufficiently close to $\pi/2$ and $\kappa = t_n^{-1}$ in (2.10).

According to (3.3), Lemma 3.1 and $\tau t_n^{-1} = \frac{1}{n} \le 1$, there exists

$$\|\mathscr{E}_\tau^n\| \le c\tau\left(\int_\kappa^{\frac{\pi}{\tau\sin\theta}} e^{rt_n\cos\theta}r^{1-\alpha}dr + \int_{-\theta}^{\theta} e^{\kappa t_n\cos\psi}\kappa^{2-\alpha}d\psi\right) \le c\tau t_n^{\alpha-2} \le ct_n^{\alpha-1}. \tag{3.9}$$

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

$$
\begin{aligned}
(\mathscr{E}_\tau(t)*G(t))(t_n) &= \left(\sum_{j=0}^{\infty}\mathscr{E}_\tau^j\delta_{t_j}(t)*G(t)\right)(t_n)\\
&=\sum_{j=0}^{n}\mathscr{E}_\tau^jG(t_n-t_j)=\sum_{j=0}^{n}\mathscr{E}_\tau^{n-j}G(t_j)=V^n.
\end{aligned}
\tag{3.10}
$$

Moreover, using the above equation, there exist

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

From (3.7), (3.10) and (3.5), we have the following estimate

$$
\left\|\left((\mathscr{E}_\tau-\mathscr{E})*\frac{t^l}{l!}\right)(t_n)\right\|\le c\tau^{l+1}t_n^{\alpha-2}+c\tau^2t_n^{\alpha+l-3}\le c\tau^lt_n^{\alpha-1}\quad l=0,1,2.
\tag{3.11}
$$

Next, we prove the following inequality (3.12) for $t>0$

$$
\left\|\left((\mathscr{E}_\tau-\mathscr{E})*\frac{t^2}{2}\right)(t)\right\|\le c\tau^2t^{\alpha-1},\quad \forall t\in(t_{n-1},t_n).
\tag{3.12}
$$

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

$$
\begin{aligned}
\left(\mathscr{E}*\frac{t^2}{2}\right)(t) &= \left(\mathscr{E}*\frac{t^2}{2}\right)(t_n)+(t-t_n)\left(\mathscr{E}*t\right)(t_n)\\
&\quad+\frac{(t-t_n)^2}{2}\left(\mathscr{E}*1\right)(t_n)+\frac{1}{2}\int_{t_n}^{t}(t-s)^2\mathscr{E}(s)ds,
\end{aligned}
$$

which also holds for $\left(\mathscr{E}_\tau*t^2\right)(t)$. Therefore, using (3.11), it yields

$$
\left\|\left((\mathscr{E}_\tau-\mathscr{E})*\frac{t^l}{l!}\right)(t_n)\right\|\le c\tau^{l+1}t_n^{\alpha-2}+c\tau^2t_n^{\alpha+l-3}\le c\tau^lt_n^{\alpha-1}\le c\tau^lt^{\alpha-1}.
$$

According to (3.8), (2.2) and (3.6), one has

$$
\|\mathscr{E}(t)\|\le c\left(\int_{\kappa}^{\infty}e^{rt\cos\theta}r^{1-\alpha}dr+\int_{-\theta}^{\theta}e^{\kappa t\cos\psi}\kappa^{2-\alpha}d\psi\right)\le ct^{\alpha-2}.
$$

Moreover, we get

$$
\left\|\int_{t_n}^{t}(t-s)^2\mathscr{E}(s)ds\right\|\le c\int_{t}^{t_n}(s-t)^2s^{\alpha-2}ds\le c\int_{t}^{t_n}(s-t)s^{\alpha-1}ds\le c\tau^2t^{\alpha-1}.
$$

Using the definition of $\mathscr{E}_\tau(t)=\sum_{n=0}^{\infty}\mathscr{E}_\tau^n\delta_{t_n}(t)$ in (3.10) and (3.9), we deduce

$$
\left\|\int_{t_n}^{t}(t-s)^2\mathscr{E}_\tau(s)ds\right\|\le(t_n-t)^2\|\mathscr{E}_\tau^n\|\le c\tau^3t_n^{\alpha-2}\le c\tau^2t_n^{\alpha-1}\le c\tau^2t^{\alpha-1},\ \forall\, t\in(t_{n-1},t_n).
$$

By (3.11) and the above inequalities, it yields the inequality (3.12). The proof is completed. □

THEOREM 3.8 (ID1-BDF2). *Let $V(t_n)$ and V^n be the solutions of* (2.3) *and* (2.7), *respectively. Let $v \in L^2(\Omega)$, $g \in C^1([0,T]; L^2(\Omega))$ and $\int_0^t (t-s)^{\alpha-1} \|g''(s)\| \, ds < \infty$. Then the following error estimate holds for any $t_n > 0$:*

$$\|V^n - V(t_n)\| \leq c\tau^2 \left(t_n^{-2} \|v\| + t_n^{\alpha-2} \|g(0)\| + t_n^{\alpha-1} \|g'(0)\| + \int_0^{t_n} (t_n - s)^{\alpha-1} \|g''(s)\| \, ds \right).$$

Proof. Subtracting (2.9) from (2.13), we obtain

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

with

$$\begin{aligned} I_1 =& \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \left[\left(\delta_\tau^\alpha (e^{-z\tau}) - A \right)^{-1} \delta_\tau (e^{-z\tau}) \gamma_1 (e^{-z\tau}) \tau^2 - (z^\alpha - A)^{-1} z^{-1} \right] Avdz, \\ I_2 =& \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa} \setminus \Gamma_{\theta,\kappa}^\tau} e^{zt_n} (z^\alpha - A)^{-1} z^{-1} Avdz, \\ I_3 =& \frac{\tau}{2\pi i} \int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \left(\delta_\tau^\alpha (e^{-z\tau}) - A \right)^{-1} \delta_\tau (e^{-z\tau}) \widetilde{G}(e^{-z\tau}) dz \\ &- \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}} e^{zt_n} (z^\alpha - A)^{-1} z \widehat{G}(z) dz. \end{aligned}$$

According to the Lemma 3.5, we estimate the first term I_1 as following

$$\begin{aligned} \|I_1\| \leq& c\tau^2 \|v\| \int_{\Gamma_{\theta,\kappa}^\tau} \left| e^{zt_n} \right| |z| |dz| \\ \leq& c\tau^2 \|v\| \left(\int_\kappa^{\frac{\pi}{\tau \sin\theta}} e^{rt_n \cos\theta} r dr + \int_{-\theta}^{\theta} e^{\kappa t_n \cos\psi} \kappa^2 d\psi \right) \\ \leq& c\tau^2 t_n^{-2} \|v\|. \end{aligned} \tag{3.13}$$

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

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

since

$$\begin{aligned} \int_{\Gamma_{\theta,\kappa} \setminus \Gamma_{\theta,\kappa}^\tau} \left| e^{zt_n} \right| |z|^{-1} |dz| =& \int_{\frac{\pi}{\tau \sin\theta}}^\infty e^{rt_n \cos\theta} r^{-1} dr \\ &\leq c\tau^2 \int_{\frac{\pi}{\tau \sin\theta}}^\infty e^{rt_n \cos\theta} r dr \leq c\tau^2 t_n^{-2} \end{aligned} \tag{3.15}$$

with $1 \leq (\frac{\sin\theta}{\pi})^2 \tau^2 r^2$, $r\tau \geq \frac{\pi}{\sin\theta}$.

From Lemmas 3.6 and 3.7 with $G(t) = tg(0) + \frac{t^2}{2} g'(0) + \frac{t^2}{2} * g''(t)$, there exist

$$\|I_3\| \leq c\tau^2 t_n^{\alpha-2} \|g(0)\| + c\tau^2 t_n^{\alpha-1} \|g'(0)\| + c\tau^2 \int_0^{t_n} (t_n - s)^{\alpha-1} \|g''(s)\| \, ds.$$

The proof is completed. □

THEOREM 3.9 (ID2-BDF2). *Let $V(t_n)$ and V^n be the solutions of* (2.4) *and* (2.8), *respectively. Let $v \in L^2(\Omega)$, $g \in C^1([0,T];L^2(\Omega))$ and $\int_0^t (t-s)^{\alpha-1}\|g''(s)\|\,ds < \infty$. Then the following error estimate holds for any $t_n > 0$:*

$$\|V^n - V(t_n)\| \le c\tau^2 \left(t_n^{-2}\|v\| + t_n^{\alpha-2}\|g(0)\| + t_n^{\alpha-1}\|g'(0)\| + \int_0^{t_n} (t_n-s)^{\alpha-1}\|g''(s)\|\,ds \right).$$

Proof. Similar arguments can be performed as Theorem 3.8, we omit it here. □

4. Convergence analysis: Singular source function $t^\mu q(x)$, $\mu \ge -\alpha$. Form Theorem 3.8 and Theorem 3.9, it seems that there are no difference between ID1-BDF2 and ID2-BDF2 for general source function. However, both of them are very different for the singular source function with the form $t^\mu q(x)$.

4.1. Low regularity source term. In the section, we first consider low regularity source term $g(x,t) = t^\mu q(x)$ with $\mu > 0$ for subdiffusion (2.3). We introduce the polylogarithm function or Bose-Einstein integral

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

LEMMA 4.1. *[9, 32] Let $|z\tau| \le \frac{\pi}{\sin\theta}$ and $\theta > \pi/2$ be close to $\pi/2$, and $p \ne 1, 2, \ldots$. The series*

$$Li_p(e^{-z\tau}) = \Gamma(1-p)(z\tau)^{p-1} + \sum_{j=0}^{\infty} (-1)^j \zeta(p-j)\frac{(z\tau)^j}{j!} \tag{4.2}$$

converges absolutely. Here ζ denotes the Riemann zeta function, namely, $\zeta(p) = Li_p(1)$.

Let $G(t) = J^1 g(t) = \frac{t^{\mu+1}}{\mu+1}q$. Using $\widehat{G}(z) = \frac{\Gamma(\mu+1)}{z^{\mu+2}}q$ and (2.9), we have

$$V(t) = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{zt}(z^\alpha - A)^{-1}\left(z^{-1}Av + \frac{\Gamma(\mu+1)}{z^{\mu+1}}q\right)dz. \tag{4.3}$$

From (2.13), the discrete solution for the subdiffusion (2.7) is

$$V^n = \frac{1}{2\pi i}\int_{\Gamma^\tau_{\theta,\kappa}} e^{zt_n}(\delta^\alpha_\tau(e^{-z\tau}) - A)^{-1}\delta_\tau(e^{-z\tau})\tau\left(\gamma_1(e^{-z\tau})\tau Av + \widetilde{G}(e^{-z\tau})\right)dz \tag{4.4}$$

with $\gamma_1(e^{-z\tau}) = \frac{e^{-z\tau}}{(1-e^{-z\tau})^2}$ and $\Gamma^\tau_{\theta,\kappa} = \{z \in \Gamma_{\theta,\kappa} : |\Im z| \le \pi/\tau\}$. Here

$$\widetilde{G}(\xi) = \sum_{n=1}^{\infty} G^n\xi^n = q\frac{\tau^{\mu+1}}{\mu+1}\sum_{n=1}^{\infty}\frac{\xi^n}{n^{-\mu-1}} = q\frac{\tau^{\mu+1}}{\mu+1}Li_{-\mu-1}(\xi) \quad \text{with} \quad 0<\mu<1.$$

LEMMA 4.2. *Let δ^α_τ is given by* (2.6) *and $\gamma_l(\xi) = \sum_{n=1}^\infty n^l\xi^n = \left(\xi\frac{d}{d\xi}\right)^l \frac{1}{1-\xi}$ with $l = 1, 2$ are given by Lemma 3.3. Then there exist a positive constants c such that*

$$\left\|\left(\delta^\alpha_\tau(e^{-z\tau}) - A\right)^{-1}\delta^l_\tau(e^{-z\tau}) - (z^\alpha - A)^{-1}z^l\right\| \le c\tau^2|z|^{l+2-\alpha},$$

$$\left\|\left(\delta^\alpha_\tau(e^{-z\tau}) - A\right)^{-1}\delta^l_\tau(e^{-z\tau})\frac{\gamma_l(e^{-z\tau})}{l!}\tau^{l+1} - (z^\alpha - A)^{-1}z^{-1}\right\| \le c\tau^2|z|^{1-\alpha} \quad \forall z \in \Gamma^\tau_{\theta,\kappa},$$

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

Proof. First we consider

$$\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} \delta_\tau^l(e^{-z\tau}) - (z^\alpha - A)^{-1} z^l = I + II$$

with

$$I = \left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} \left(\delta_\tau^l(e^{-z\tau}) - z^l\right),$$
$$II = \left(\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} - (z^\alpha - A)^{-1}\right) z^l.$$

According to (3.3) and Lemma 3.1, we obtain

$$\|I\| \leq c\tau^2 |z|^{l+2-\alpha}.$$

Using the Lemma 3.1, (3.3), (2.2) and the identity

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

we estimate II as following

$$\|II\| \leq c\tau^2 |z|^{2+\alpha} c|z|^{-\alpha} c|z|^{-\alpha} |z|^l \leq c\tau^2 |z|^{l+2-\alpha}.$$

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

Next we consider

$$\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} \delta_\tau^l(e^{-z\tau}) \frac{\gamma_l(e^{-z\tau})}{l!} \tau^{l+1} - (z^\alpha - A)^{-1} z^{-1} = J_1 + J_2$$

with

$$J_1 = \left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} \delta_\tau^l(e^{-z\tau}) \left[\frac{\gamma_l(e^{-z\tau})}{l!} \tau^{l+1} - z^{-l-1}\right],$$
$$J_2 = \left[\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} \delta_\tau^l(e^{-z\tau}) - (z^\alpha - A)^{-1} z^l\right] z^{-l-1}.$$

According to (3.3) and Lemmas 3.1, 3.2 with $l = 1, 2$, we obtain

$$\|J_1\| \leq c\tau^{l+1} |z|^{l-\alpha} \leq c\tau^2 |z|^{1-\alpha}.$$

From I and II, we have

$$\|J_2\| \leq c\tau^2 |z|^{l+2-\alpha} |z|^{-l-1} = c\tau^2 |z|^{1-\alpha}.$$

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

LEMMA 4.3. *Let $\widehat{G}(z) = \frac{1}{\mu+1} \frac{\Gamma(\mu+2)}{z^{\mu+2}} q$ and $\widetilde{G}(e^{-z\tau}) = q \frac{\tau^{\mu+1}}{\mu+1} Li_{-\mu-1}(e^{-z\tau})$. Then*

$$\left\|\tau \widetilde{G}(e^{-z\tau}) - \widehat{G}(z)\right\| \leq c\tau^{\mu+2} \|q\|, \quad \mu \notin \mathbb{N}.$$

Proof. Using the definitions of $\widehat{G}(z)$ and $\widetilde{G}(e^{-z\tau})$ and Lemma 4.1 with $p = -\mu - 1$, we have

$$\begin{aligned}\left\|\tau \widetilde{G}(e^{-z\tau}) - \widehat{G}(z)\right\| &= \left\|\frac{\tau^{\mu+2}}{(\mu+1)} \left(Li_{-\mu-1}(e^{-z\tau}) - \frac{\Gamma(\mu+2)}{(z\tau)^{\mu+2}}\right) q\right\| \\ &\leq \frac{\tau^{\mu+2}}{(\mu+1)} \left|\sum_{j=0}^{\infty} (-1)^j \zeta(-\mu - 1 - j) \frac{(z\tau)^j}{j!}\right| \|q\| \leq c\tau^{\mu+2} \|q\|.\end{aligned}$$

The proof is completed. ∎

THEOREM 4.4 (ID1-BDF2). *Let $V(t_n)$ and V^n be the solutions of (2.3) and (2.7), respectively. Let $v \in L^2(\Omega)$ and $g(x,t) = t^\mu q(x)$, $\mu > 0$, $q(x) \in L^2(\Omega)$. Then*

$$\|V^n - V(t_n)\| \leq c\tau^2 t_n^{-2}\|v\| + c\tau^{\mu+2} t_n^{\alpha-2}\|q\| + c\tau^2 t_n^{\alpha+\mu-2}\|q\|.$$

Proof. From Theorem 3.8, the desired results is obtained with $\mu \in \mathbb{N}$. We next prove the case $\mu \notin \mathbb{N}$. Subtracting (4.3) from (4.4), we obtain

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

with

$$\begin{aligned}
I_1 =& \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\left[\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\delta_\tau(e^{-z\tau})\gamma_1(e^{-z\tau})\tau^2 - (z^\alpha - A)^{-1}z^{-1}\right]Avdz,\\
I_2 =& \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}\setminus\Gamma_{\theta,\kappa}^\tau} e^{zt_n}(z^\alpha - A)^{-1}z^{-1}Avdz,\\
I_3 =& \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n}\left[\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1}\delta_\tau(e^{-z\tau})\tau\widetilde{G}(e^{-z\tau}) - (z^\alpha - A)^{-1}z\widehat{G}(z)\right]dz,\\
I_4 =& \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}\setminus\Gamma_{\theta,\kappa}^\tau} e^{zt_n}(z^\alpha - A)^{-1}z\widehat{G}(z)dz.
\end{aligned}$$

According to (3.13) and (3.14), we estimate I_1 and I_2 as following

$$\|I_1\| \leq c\tau^2 t_n^{-2}\|v\| \quad \text{and} \quad \|I_2\| \leq c\tau^2 t_n^{-2}\|v\|.$$

From (3.15), we estimate that I_4 is similar to I_2 as following

$$\begin{aligned}
\|I_4\| \leq& c\int_{\Gamma_{\theta,\kappa}\setminus\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right||z|^{-\alpha}\left\|z\widehat{G}(z)\right\||dz|\\
\leq& c\int_{\Gamma_{\theta,\kappa}\setminus\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right||z|^{-\alpha}|z|^{-\mu-1}\|q\||dz| \leq c\tau^2 t_n^{\alpha+\mu-2}\|q\|.
\end{aligned}$$

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

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

According to (3.3) and Lemmas 3.1 and 4.3, there exists

$$\|I_{31}\| \leq c\tau^{\mu+2}\|q\|\int_{\Gamma_{\theta,\kappa}^\tau}\left|e^{zt_n}\right||z|^{1-\alpha}|dz| \leq c\tau^{\mu+2}t_n^{\alpha-2}\|q\|.$$

From Lemma 4.2 and $\widehat{G}(z) = \frac{1}{\mu+1}\frac{\Gamma(\mu+2)}{z^{\mu+2}}q$, we estimate I_{32} as following

$$\|I_{32}\| \leq c\tau^2\|q\|\int_{\Gamma_{\theta,\kappa}^\tau}\left|e^{zt_n}\right||z|^{3-\alpha}|z|^{-\mu-2}|dz| \leq c\tau^2 t_n^{\alpha+\mu-2}\|q\|.$$

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

4.2. Singular source term. In this subsection, we consider the singular source term $g(x,t)=t^{\mu}q(x)$ with $\mu\geq -\alpha$ for subdiffusion (2.4).

Let $\mathcal{G}(t)=J^2g(t)=\frac{t^{\mu+2}}{(\mu+1)(\mu+2)}q$. Using $\widehat{\mathcal{G}}(z)=\frac{\Gamma(\mu+1)}{z^{\mu+3}}q$ and (2.11), we have

$$V(t)=\frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}}e^{zt}(z^{\alpha}-A)^{-1}\left(z^{-1}Av+\frac{\Gamma(\mu+1)}{z^{\mu+1}}q\right)dz. \tag{4.5}$$

From (2.15), it yields

$$V^n=\frac{\tau}{2\pi i}\int_{\Gamma^{\tau}_{\theta,\kappa}}e^{zt_n}\left(\delta_{\tau}^{\alpha}(e^{-z\tau})-A\right)^{-1}\delta_{\tau}^{2}(e^{-z\tau})\left(\frac{\gamma_2(e^{-z\tau})}{2}\tau^2Av+\widetilde{\mathcal{G}}(e^{-z\tau})\right)dz$$

with $\frac{\gamma_2(e^{-z\tau})}{2}=\frac{e^{-z\tau}+e^{-2z\tau}}{2(1-e^{-z\tau})^3}$ and $\Gamma^{\tau}_{\theta,\kappa}=\{z\in\Gamma_{\theta,\kappa}:|\Im z|\leq \pi/\tau\}$. Here

$$\widetilde{\mathcal{G}}(\xi)=\sum_{n=1}^{\infty}\mathcal{G}^n\xi^n=q\frac{\tau^{\mu+2}}{(\mu+2)(\mu+1)}\sum_{n=1}^{\infty}\frac{\xi^n}{n^{-\mu-2}}=q\frac{\tau^{\mu+2}}{(\mu+2)(\mu+1)}Li_{-\mu-2}(\xi).$$

Lemma 4.5. *Let* $\widehat{\mathcal{G}}(z)=q\frac{\Gamma(\mu+1)}{z^{\mu+3}}$ *and* $\widetilde{\mathcal{G}}(e^{-z\tau})=q\frac{\tau^{\mu+2}}{(\mu+2)(\mu+1)}Li_{-\mu-2}(e^{-z\tau})$. *Then*

$$\left\|\tau\widetilde{\mathcal{G}}(e^{-z\tau})-\widehat{\mathcal{G}}(z)\right\|\leq c\tau^{\mu+3}\left\|q\right\|,\quad \mu\notin\mathbb{N}.$$

Proof. From Lemma 4.1, we have

$$\begin{aligned}\left\|\tau\widetilde{\mathcal{G}}(e^{-z\tau})-\widehat{\mathcal{G}}(z)\right\|=&\left\|\frac{\tau^{\mu+3}}{(\mu+2)(\mu+1)}\left(Li_{-\mu-2}(e^{-z\tau})-\frac{\Gamma(\mu+3)}{(z\tau)^{\mu+3}}\right)q\right\|\\ \leq&\frac{\tau^{\mu+3}}{(\mu+2)(\mu+1)}\left|\sum_{j=0}^{\infty}(-1)^j\zeta(-\mu-2-j)\frac{(z\tau)^j}{j!}\right|\left\|q\right\|\\ \leq& c\tau^{\mu+3}\left\|q\right\|.\end{aligned}$$

The proof is completed. □

Theorem 4.6 (ID2-BDF2). *Let* $V(t_n)$ *and* V^n *be the solutions of* (2.4) *and* (2.8), *respectively. Let* $v\in L^2(\Omega)$ *and* $g(x,t)=t^{\mu}q(x)$, $\mu\geq-\alpha$, $q(x)\in L^2(\Omega)$. *Then*

$$\|V^n-V(t_n)\|\leq c\tau^2t_n^{-2}\|v\|+c\tau^{\mu+3}t_n^{\alpha-3}\left\|q\right\|+c\tau^2t_n^{\alpha+\mu-2}\left\|q\right\|.$$

Proof. From Theorem 3.8, the desired results is obtained with $\mu\in\mathbb{N}$. We next prove the case $\mu\notin\mathbb{N}$. Subtracting (2.11) from (2.15), we obtain

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

with

$$\begin{aligned}I_1=&\frac{1}{2\pi i}\int_{\Gamma^{\tau}_{\theta,\kappa}}e^{zt_n}\left[\left(\delta_{\tau}^{\alpha}(e^{-z\tau})-A\right)^{-1}\delta_{\tau}^{2}(e^{-z\tau})\frac{e^{-z\tau}+e^{-2z\tau}}{2(1-e^{-z\tau})^3}\tau^3-(z^{\alpha}-A)^{-1}z^{-1}\right]Avdz,\\ I_2=&\frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}\backslash\Gamma^{\tau}_{\theta,\kappa}}e^{zt_n}(z^{\alpha}-A)^{-1}z^{-1}Avdz,\\ I_3=&\frac{1}{2\pi i}\int_{\Gamma^{\tau}_{\theta,\kappa}}e^{zt_n}\left[\left(\delta_{\tau}^{\alpha}(e^{-z\tau})-A\right)^{-1}\delta_{\tau}^{2}(e^{-z\tau})\tau\widetilde{\mathcal{G}}(e^{-z\tau})-(z^{\alpha}-A)^{-1}z^2\widehat{\mathcal{G}}(z)\right]dz,\\ I_4=&\frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}\backslash\Gamma^{\tau}_{\theta,\kappa}}e^{zt_n}(z^{\alpha}-A)^{-1}z^2\widehat{\mathcal{G}}(z)dz.\end{aligned}$$

Using (3.13), (3.14) and Lemma 4.2, we estimate I_1 and I_2 as following

$$\|I_1\| \le c\tau^2 t_n^{-2} \|v\| \quad \text{and} \quad \|I_2\| \le c\tau^2 t_n^{-2} \|v\|.$$

By (3.15), we estimate that I_4 is similar to I_2 as following

$$\begin{aligned}\|I_4\| &\le c \int_{\Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right| |z|^{-\alpha} \left\|z^2\widehat{\mathcal{G}}(z)\right\| |dz| \\ &\le c\|q\| \int_{\Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right| |z|^{-\alpha}|z|^{-\mu-1}|dz| \le c\tau^2 t_n^{\alpha+\mu-2}\|q\|.\end{aligned}$$

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

$$\begin{aligned}I_{31} =& \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} \delta_\tau^2(e^{-z\tau}) \left(\tau\widetilde{\mathcal{G}}(e^{-z\tau}) - \widehat{\mathcal{G}}(z)\right) dz, \\ I_{32} =& \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}^\tau} e^{zt_n} \left(\left(\delta_\tau^\alpha(e^{-z\tau}) - A\right)^{-1} \delta_\tau^2(e^{-z\tau}) - (z^\alpha - A)^{-1} z^2\right) \widehat{\mathcal{G}}(z) dz.\end{aligned}$$

According to (3.3) and Lemmas 3.1 and 4.5, there exists

$$\|I_{31}\| \le c\tau^{\mu+3}\|q\| \int_{\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right| |z|^{2-\alpha}|dz| \le c\tau^{\mu+3} t_n^{\alpha-3}\|q\|.$$

From Lemma 4.2, we estimate I_{32} as following

$$\begin{aligned}\|I_{32}\| \le& c\tau^2\|q\| \int_{\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right| |z|^{4-\alpha}|z|^{-\mu-3}|dz| \\ \le& c\tau^2\|q\| \int_{\Gamma_{\theta,\kappa}^\tau} \left|e^{zt_n}\right| |z|^{1-\alpha-\mu}|dz| \le c\tau^2 t_n^{\alpha+\mu-2}\|q\|.\end{aligned}$$

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

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

Based on the discussion of Section 3 and 4, we now analyse the error estimates for subdiffusion (1.1) with the singular source term $t^\mu \circ f(x,t)$.

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

Let $f(t) = f(0) + tf'(0) + t * f''(t)$. Then we obtain

$$g(t) = t^\mu * f(t) = \frac{t^{\mu+1}f(0)}{\mu+1} + \frac{t^{\mu+2}f'(0)}{(\mu+1)(\mu+2)} + t^\mu * t * f''(t).$$

Let $G(t) = J^1 g(t) = \frac{1}{\mu+1}t^{\mu+1} * f(t)$ with $G(0) = 0$. It yields

$$\begin{aligned}G(t) &= \frac{t^{\mu+2}f(0)}{(\mu+1)(\mu+2)} + \frac{t^{\mu+3}f'(0)}{(\mu+1)(\mu+2)(\mu+3)} + \frac{1}{\mu+1}t^{\mu+1} * t * f''(t) \\ &= \frac{t^{\mu+2}f(0)}{(\mu+1)(\mu+2)} + \frac{t^{\mu+3}f'(0)}{(\mu+1)(\mu+2)(\mu+3)} + \frac{t^2}{2} * (t^\mu * f''(t)),\end{aligned}$$

where we use

$$t^{\mu+1} * t = \int_0^t (t-s)^{\mu+1} s ds = \frac{\mu+1}{2}\int_0^t (t-s)^\mu s^2 ds = \frac{\mu+1}{2} t^2 * t^\mu.$$

LEMMA 5.1. *Let $V(t_n)$ and V^n be the solutions of* (2.3) *and* (2.7)*, respectively. Let $v=0$, $G(t):=\frac{t^2}{2}*(t^\mu * f''(t))$ with $\mu>-1$ and $\int_0^t (t-s)^{\alpha-1}s^\mu * \|f''(s)\|\,ds<\infty$. Then*

$$\|V(t_n)-V^n\| \le c\tau^2 \int_0^{t_n} (t_n-s)^{\alpha-1}s^\mu * \|f''(s)\|\,ds \le c\tau^2 \int_0^{t_n} (t_n-s)^{\alpha+\mu}\,\|f''(s)\|\,ds.$$

Proof. By Lemma 3.7 with $g''(t)=t^\mu * f''(t)$, we obtain

$$\begin{aligned}\|V(t_n)-V^n\| &\le c\tau^2 \int_0^{t_n} (t_n-s)^{\alpha-1}\,\|s^\mu * f''(s)\|\,ds\\ &\le c\tau^2 \int_0^{t_n} (t_n-s)^{\alpha-1}s^\mu * \|f''(s)\|\,ds\\ &= c\tau^2 \left(t^{\alpha-1}*t^\mu\right) * \|f''(t)\|_{t=t_n} \le c\tau^2 \int_0^{t_n} (t_n-s)^{\alpha+\mu}\,\|f''(s)\|\,ds.\end{aligned}$$

The proof is completed. ◻

THEOREM 5.2 (ID1-BDF2). *Let $V(t_n)$ and V^n be the solutions of* (2.3) *and* (2.7)*, respectively. Let $v\in L^2(\Omega)$, $g(t)=t^\mu * f(t)$ with $\mu>-1$ and $f\in C^1([0,T];L^2(\Omega))$, $\int_0^t (t-s)^{\alpha-1}s^\mu * \|f''(s)\|\,ds<\infty$. Then*

$$\begin{aligned}&\|V^n-V(t_n)\|\\ &\le c\tau^2\left(t_n^{-2}\|v\| + t_n^{\alpha+\mu-1}\,\|f(0)\| + t_n^{\alpha+\mu}\,\|f'(0)\| + \int_0^{t_n}(t_n-s)^{\alpha-1}s^\mu * \|f''(s)\|\,ds\right)\\ &\le c\tau^2\left(t_n^{-2}\|v\| + t_n^{\alpha+\mu-1}\,\|f(0)\| + t_n^{\alpha+\mu}\,\|f'(0)\| + \int_0^{t_n}(t_n-s)^{\alpha+\mu}\,\|f''(s)\|\,ds\right).\end{aligned}$$

Proof. According to Theorem 4.4, Lemma 5.1, and similar treatment of the initial data v in Theorem 3.8, the desired result is obtained. ◻

5.2. Convergence analysis: product source function $t^\mu f(t)$, $\mu>0$. Let $G(t)=J^1 g(t)$ and $f(t)=f(0)+tf'(0)+t*f''(t)$. Then we have

$$G(t)=1*(t^\mu f(t))=\frac{t^{\mu+1}f(0)}{\mu+1}+\frac{t^{\mu+2}f'(0)}{\mu+2}+1*\left[t^\mu\left(t*f''(t)\right)\right].$$

Let $h(t)=t^\mu\left(t*f''(t)\right)$ with $h(0)=0$. It leads to

$$h'(t)=\mu t^{\mu-1}\left(t*f''(t)\right)+t^\mu\left(1*f''(t)\right)$$

with $h'(0)=0$, since

$$|h'(t)|\le\left|\mu t^{\mu-1}\int_0^t (t-s)f''(s)ds\right|+\left|t^\mu\int_0^t f''(s)ds\right|\le(\mu+1)t^\mu\int_0^t|f''(s)|\,ds,\ \mu>0.$$

Moreover, there exists

$$h''(t)=\mu\left(\mu-1\right)t^{\mu-2}\left(t*f''(t)\right)+2\mu t^{\mu-1}\left(1*f''(t)\right)+t^\mu f''(t). \tag{5.1}$$

Thus one has

$$1*h(t)=th(0)+\frac{t^2}{2}h'(0)+\frac{t^2}{2}*h''(t)=\frac{t^2}{2}*h''(t). \tag{5.2}$$

LEMMA 5.3. *Let $V(t_n)$ and V^n be the solutions of* (2.3) *and* (2.7), *respectively. Let $v = 0$, $G(t) = 1 * [t^\mu (t * f''(t))]$ with $\mu > 0$ and $f \in C^1([0,T]; L^2(\Omega))$, $\int_0^t \|f''(s)\| ds < \infty$, $\int_0^t (t-s)^{\alpha-1} s^\mu \|f''(s)\| ds < \infty$. Then*

$$\|V(t_n) - V^n\| \le c\tau^2 \left(t_n^{\alpha+\mu-1} \int_0^{t_n} \|f''(s)\| ds + \int_0^{t_n} (t_n - s)^{\alpha-1} s^\mu \|f''(s)\| ds \right).$$

Proof. Let $h(t) = t^\mu (t * f''(t))$. From (5.2), we have $G(t) = 1 * h(t) = \frac{t^2}{2} * h''(t)$. According to Lemma 3.7 and (5.1), it yields

$$\|V(t_n) - V^n\| \le c\tau^2 \int_0^{t_n} (t_n - s)^{\alpha-1} \|h''(s)\| ds \le c\tau^2 (I_1 + I_2 + I_3)$$

with

$$I_1 = \int_0^{t_n} (t_n - s)^{\alpha-1} \left\| s^{\mu-2} (s * f''(s)) \right\| ds,$$
$$I_2 = \int_0^{t_n} (t_n - s)^{\alpha-1} \left\| s^{\mu-1} (1 * f''(s)) \right\| ds \quad \text{and} \quad I_3 = \int_0^{t_n} (t_n - s)^{\alpha-1} \|s^\mu f''(s)\| ds.$$

We estimate I_1 as following

$$\begin{aligned} I_1 &= \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu-1} \left\| \int_0^s \frac{s-w}{s} f''(w) dw \right\| ds \\ &\le \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu-1} \int_0^{t_n} \|f''(w)\| dw ds = B(\alpha,\mu) t_n^{\alpha+\mu-1} \int_0^{t_n} \|f''(w)\| dw, \end{aligned}$$

since

$$\int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu-1} ds = t_n^{\alpha+\mu-1} \int_0^1 (1-s)^{\alpha-1} s^{\mu-1} ds = B(\alpha,\mu) t_n^{\alpha+\mu-1}.$$

Similarly, we estimate I_2 as following

$$I_2 \le \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu-1} \int_0^{t_n} \|f''(w)\| dw ds = B(\alpha,\mu) t_n^{\alpha+\mu-1} \int_0^{t_n} \|f''(w)\| dw.$$

By the triangle inequality, we obtain

$$\|V(t_n) - V^n\| \le c\tau^2 \left(t_n^{\alpha+\mu-1} \int_0^{t_n} \|f''(s)\| ds + \int_0^{t_n} (t_n - s)^{\alpha-1} s^\mu \|f''(s)\| ds \right).$$

The proof is completed. ∎

THEOREM 5.4 (ID1-BDF2). *Let $V(t_n)$ and V^n be the solutions of* (2.3) *and* (2.7), *respectively. Let $v \in L^2(\Omega)$, $g(t) = t^\mu f(t)$ with $\mu > 0$ and $f \in C^1([0,T]; L^2(\Omega))$, $\int_0^t \|f''(s)\| ds < \infty$, $\int_0^t (t-s)^{\alpha-1} s^\mu \|f''(s)\| ds < \infty$. Then*

$$\begin{aligned} \|V^n - V(t_n)\| \le\ & c\tau^2 \left(t_n^{-2} \|v\| + t_n^{\alpha+\mu-2} \|f(0)\| + t_n^{\alpha+\mu-1} \|f'(0)\| \right) \\ & + c\tau^2 \left(t_n^{\alpha+\mu-1} \int_0^{t_n} \|f''(s)\| ds + \int_0^{t_n} (t_n - s)^{\alpha-1} s^\mu \|f''(s)\| ds \right). \end{aligned}$$

Proof. According to Theorem 4.4, Lemma 5.3, and similar treatment of the initial data v in Theorem 3.8, the desired result is obtained. ∎

5.3. Convergence analysis: product source function $t^\mu f(t)$, $-\alpha \le \mu < 0$. Let $\mathcal{G}(t) = J^2 g(t)$ and $f(t) = f(0) + tf'(0) + t * f''(t)$. Then we have

$$\mathcal{G}(t) = t * (t^\mu f(t)) = \frac{t^{\mu+2} f(0)}{(\mu+1)(\mu+2)} + \frac{t^{\mu+3} f'(0)}{(\mu+2)(\mu+3)} + t * [t^\mu (t * f''(t))].$$

Let $h(t) = t^\mu (t * f''(t))$ with $h(0) = 0$. It leads to

$$h'(t) = \mu t^{\mu-1} (t * f''(t)) + t^\mu (1 * f''(t)),$$

which implies

$$|h'(0)| \le (\mu+1) \int_0^t s^\mu |f''(s)| \, ds,$$

since

$$|h'(t)| \le (\mu+1) t^\mu \int_0^t |f''(s)| \, ds \le (\mu+1) \int_0^t s^\mu |f''(s)| \, ds \quad \text{with } -1 < \mu < 0.$$

Thus we get

$$t * h(t) = \frac{t^2}{2} h(0) + \frac{t^3}{6} h'(0) + \frac{t^3}{6} * h''(t) = \frac{t^3}{6} h'(0) + \frac{t^3}{6} * h''(t). \tag{5.3}$$

Lemma 5.5. *Let $V(t_n)$ and V^n be the solutions of (2.4) and (2.8), respectively. Let $v = 0$, $\mathcal{G}(t) = t * [t^\mu (t * f''(t))]$ with $-\alpha \le \mu < 0$ and $f \in C^1([0,T]; L^2(\Omega))$, $\int_0^t s^{\frac{\mu-1}{2}} \|f''(s)\| \, ds < \infty$, $\int_0^t (t-s)^{\alpha-1} s^\mu \|f''(s)\| \, ds$. Then*

$$\|V(t_n) - V^n\| \le c\tau^2 \left(t_n^{\alpha + \frac{\mu-1}{2}} \int_0^{t_n} s^{\frac{\mu-1}{2}} \|f''(s)\| \, ds + \int_0^{t_n} (t_n - s)^{\alpha-1} s^\mu \|f''(s)\| \, ds \right).$$

Proof. Let $h(t) = t^\mu (t * f''(t))$. From (5.3), we have

$$\mathcal{G}(t) = t * h(t) = \frac{t^3}{6} h'(0) + \frac{t^3}{6} * h''(t).$$

According to Theorems 4.6, 3.9 and (5.1), it yields

$$\begin{aligned} \|V(t_n) - V^n\| &\le c\tau^2 \left(t_n^{\alpha-1} \|h'(0)\| + \int_0^{t_n} (t_n - s)^{\alpha-1} \|h''(s)\| \, ds \right) \\ &\le c\tau^2 (I_1 + I_2 + I_3 + I_4) \end{aligned}$$

with

$$I_1 = t_n^{\alpha-1} \|h'(0)\|, \quad I_2 = \int_0^{t_n} (t_n - s)^{\alpha-1} \left\| s^{\mu-2} (s * f''(s)) \right\| ds,$$

$$I_3 = \int_0^{t_n} (t_n - s)^{\alpha-1} \left\| s^{\mu-1} (1 * f''(s)) \right\| ds \quad \text{and} \quad I_4 = \int_0^{t_n} (t_n - s)^{\alpha-1} \|s^\mu f''(s)\| \, ds.$$

Since

$$I_1 = t_n^{\alpha-1} \|h'(0)\| \le c t_n^{\alpha-1} \int_0^{t_n} s^\mu \|f''(s)\| \, ds \le c \int_0^{t_n} (t_n - s)^{\alpha-1} s^\mu \|f''(s)\| \, ds,$$

and

$$I_2 = \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\frac{\mu-1}{2}} \left\| \int_0^s \frac{s-w}{s} s^{\frac{\mu-1}{2}} f''(w) dw \right\| ds$$
$$\leq \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\frac{\mu-1}{2}} \int_0^{t_n} w^{\frac{\mu-1}{2}} \|f''(w)\| dw ds \leq c t_n^{\alpha+\frac{\mu-1}{2}} \int_0^{t_n} w^{\frac{\mu-1}{2}} \|f''(w)\| dw,$$

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 estimate I_3 as following

$$I_3 \leq \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu-1} \int_0^{t_n} \|f''(w)\| dw ds \leq c t_n^{\alpha+\frac{\mu-1}{2}} \int_0^{t_n} w^{\frac{\mu-1}{2}} \|f''(w)\| dw.$$

By the triangle inequality, we obtain

$$\|V(t_n) - V^n\| \leq c\tau^2 \left(t_n^{\alpha+\frac{\mu-1}{2}} \int_0^{t_n} s^{\frac{\mu-1}{2}} \|f''(s)\| ds + \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu} \|f''(s)\| ds \right).$$

The proof is completed. □

THEOREM 5.6 (ID2-BDF2). *Let $V(t_n)$ and V^n be the solutions of* (2.4) *and* (2.8)*, respectively. Let $v \in L^2(\Omega)$, $g(t) = t^{\mu} f(t)$ with $-\alpha \leq \mu < 0$ and $f \in C^1([0,T]; L^2(\Omega))$, $\int_0^t s^{\frac{\mu-1}{2}} \|f''(s)\| ds < \infty$, $\int_0^t (t-s)^{\alpha-1} s^{\mu} \|f''(s)\| ds$. Then*

$$\|V^n - V(t_n)\| \leq c\tau^2 \left(t_n^{-2} \|v\| + t_n^{\alpha+\mu-2} \|f(0)\| + t_n^{\alpha+\mu-1} \|f'(0)\| \right)$$
$$+ c\tau^2 \left(t_n^{\alpha+\frac{\mu-1}{2}} \int_0^{t_n} s^{\frac{\mu-1}{2}} \|f''(s)\| ds + \int_0^{t_n} (t_n - s)^{\alpha-1} s^{\mu} \|f''(s)\| ds \right).$$

Proof. According to Theorem 4.6, Lemma 5.5, and similar treatment of the initial data v in Theorem 3.8, the desired result is obtained. □

REMARK 5.1. *Theorems 4.6 and 5.6 are naturally extended to $\mu > -1$.*

6. Numerical results. We numerically verify the above theoretical results and the discrete L^2-norm is used to measure the numerical errors. In the space direction, it is discretized with the spectral collocation method with the Chebyshev-Gauss-Lobatto points [25]. Here we main focus on the time direction convergence order, since the convergence rate of the spatial discretization is well understood. Since the analytic solutions is unknown, the order of the convergence of the numerical results are computed by the following formula

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

with $u^N = V^N + v$ in (2.7).

In the experiment, several algorithms including the correction BDF2 methods [10] are carried out and compared with IDk-mehtod:

$$\text{BDF2 Method}: \quad \partial_\tau^\alpha V^n - AV^n = Av + g^n. \tag{6.1}$$

$$\text{(6.2)} \qquad \text{Corr}-\text{BDF2 Method}: \quad \partial_\tau^\alpha V^n - AV^n = \frac{3}{2}Av + \frac{1}{2}g^0 + g^n.$$

EXAMPLE 6.1. *Let $T = 1$ and $\Omega = (-1, 1)$. Consider subdiffusion* (1.1) *with*

$$v(x) = \sin(x)\sqrt{1-x^2} \quad \text{and} \quad g(x,t) = (1 + t^\mu + t^{\alpha\mu}) \circ (1-t)^\beta e^x (1 + \chi_{(0,1)}(x)).$$

Here $J^k g(x,t) = t^{k-1} * g(x,t)$, $k = 1, 2$ are calculated by JacobiGL Algorithm [2, 7], which is generating the nodes and weights of Gauss-Labatto integral with the weighting function such as $(1-t)^\mu$ or $(1+t)^\mu$.

Table 6.1: The discrete L^2-norm $||u^N - u^{2N}||$ and convergent order of schemes (6.1), (6.2) and (2.7), (2.8) with $\beta = 0$, $\alpha = 0.7$. Here $\circ$ denotes the dot product.

Scheme	μ	$N = 50$	$N = 100$	$N = 200$	$N = 400$	$N = 800$
BDF2	0.8	2.4743e-03	1.1981e-03	5.8732e-04	2.9005e-04	1.4390e-04
			1.0462	1.0286	1.0178	1.0113
	-0.8	1.5948e-01	1.3256e-01	1.1109e-01	9.3707e-02	7.9450e-02
			0.26679	0.25489	0.24549	0.23811
Corr-BDF2	0.8	9.4381e-05	3.6107e-05	1.3189e-05	4.6888e-06	1.6386e-06
			1.3862	1.4529	1.4921	1.5168
	-0.8	NaN	NaN	NaN	NaN	NaN
ID1-BDF2	0.8	1.6660e-04	4.1216e-05	1.0249e-05	2.5553e-06	6.3792e-07
			2.0151	2.0077	2.0040	2.0021
	-0.8	6.7744e-03	3.0380e-03	1.3367e-03	5.8281e-04	2.5299e-04
			1.1570	1.1844	1.1976	1.2039
ID2-BDF2	0.8	3.2389e-04	7.9995e-05	1.9879e-05	4.9539e-06	1.2374e-06
			2.0175	2.0087	2.0046	2.0013
	-0.8	2.1611e-03	5.2769e-04	1.3018e-04	3.2292e-05	8.0280e-06
			2.0340	2.0192	2.0112	2.0081

For subdiffusion PDEs model (1.1), it is natural appearing the low regularity/singular term such as

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

In this case, many popular time stepping schemes, including the correction of high-order BDF methods may lose their high-order accuracy, see [10, Section 4.1] and Lemma 3.2 in [31], also see Table 6.1. The correction BDF2 methods recovers super-linear convergence order $\mathcal{O}(\tau^{1+\alpha\mu})$, provided that the source term behaves like $t^{\alpha\mu}$, which is invalid for $\mu < 0$, since it is required the source function $g \in C([0,T]; L^2(\Omega))$.

To fill in this gap, the desired second-order convergence rate can be achieved by ID1-BDF2 with $\mu > 0$ but it is still likely to exhibit a order reduction with $\mu < 0$. Furthermore, ID2-BDF2 method has filled a gap with $-1 < \mu < 0$, see Tables 6.1 and 6.2. Tables 6.3 shows that ID1-BDF2 recovers second order convergence and this is in agreement with the order of the convergence for $t^\mu * f(x,t)$, $\mu > -1$.

REMARK 6.1. *For Hadamard's finite-Part integral [6, p. 233]*

$$\int_0^t s^\mu ds = \frac{1}{1+\mu} t^{1+\mu}, \ \mu < -1,$$

Table 6.2: The discrete L^2-norm $||u^N - u^{2N}||$ and convergent order of schemes (2.7) and (2.8) with $\beta = 1.9$, respectively. Here $\circ$ denotes the dot product.

Scheme	α	μ	$N=50$	$N=100$	$N=200$	$N=400$	$N=800$
ID1-BDF2	0.3	0.5	1.5025e-03	3.9778e-04	1.0433e-04	2.7198e-05	7.0660e-06
				1.9174	1.9307	1.9396	1.9445
		-0.9	4.9903e-03	2.7664e-03	1.4020e-03	6.8259e-04	3.2574e-04
				0.85109	0.98050	1.0384	1.0673
	0.7	0.5	6.8462e-04	1.8033e-04	4.6484e-05	1.1840e-05	2.9948e-06
				1.9247	1.9558	1.9731	1.9831
		-0.9	2.0722e-02	1.0219e-02	4.8849e-03	2.3017e-03	1.0770e-03
				1.0199	1.0648	1.0856	1.0956
ID2-BDF2	0.3	0.5	3.1810e-03	8.4340e-04	2.2164e-04	5.7938e-05	1.5180e-05
				1.9152	1.9280	1.9356	1.9323
		-0.9	4.6179e-03	1.1806e-03	3.0298e-04	7.7857e-05	2.0182e-05
				1.9677	1.9622	1.9603	1.9478
	0.7	0.5	1.9266e-03	5.0536e-04	1.3015e-04	3.3167e-05	8.4027e-06
				1.9307	1.9571	1.9724	1.9808
		-0.9	7.2846e-03	1.8010e-03	4.4808e-04	1.1179e-04	2.7922e-05
				2.0161	2.0070	2.0030	2.0013

Table 6.3: The discrete L^2-norm $||u^N - u^{2N}||$ and convergent order of schemes (6.1) and (2.7) with $\beta = 1.9$, respectively. Here $\circ$ denotes the Laplace convolution.

Scheme	α	μ	$N=50$	$N=100$	$N=200$	$N=400$	$N=800$
ID1-BDF2	0.3	-0.2	6.4420e-05	1.2431e-05	2.6710e-06	6.1586e-07	1.4766e-07
				2.3735	2.2185	2.1167	2.0603
		-0.8	1.6132e-03	4.2435e-04	1.0992e-04	2.8213e-05	7.2033e-06
				1.9266	1.9487	1.9621	1.9696
	0.7	-0.2	2.8145e-04	6.7873e-05	1.6649e-05	4.1218e-06	1.0253e-06
				2.0520	2.0274	2.0141	2.0072
		-0.8	6.3566e-04	1.7068e-04	4.4407e-05	1.1358e-05	2.8782e-06
				1.8969	1.9425	1.9671	1.9805

of course the limit does not exist, and so Hadamard suggested simply to ignore the unbounded contribution. In this case, we can similar provide

$$\mathrm{ID3-BDF2\ Method}: \partial_\tau^\alpha V^n - AV^n = \partial_\tau^3\left(\frac{t_n^3}{6}Av + \mathbb{G}^n\right),\ \mathbb{G} = J^3 g(x,t),$$

which also recovers the high-order accuracy even for the hypersingul source term, see Table 6.4.

7. Conclusions. Fractional PDEs model naturally imply a less smooth or low regularity source function $t^\mu \circ f(x,t)$ in the right-hand side, which is likely to result in a severe order reduction in most existing time-stepping schemes. To fill in this gap, we provides a new idea to obtain the second-order time-stepping schemes for subdiffusion, called IDk-BDF2 method. The detailed theoretical analysis and numerical verifications are presented. In the future studies, we will try to adapt the idea to higher order schemes and the nonlinear fractional models [12].

Table 6.4: The discrete L^2-norm $||u^N - u^{2N}||$ and convergent order with $\beta = 0$, $\alpha = 0.7$. Here $\circ$ denotes the dot product.

Scheme	μ	$N = 50$	$N = 100$	$N = 200$	$N = 400$	$N = 800$
ID2-BDF2	-1.8	1.7275e-02	8.1527e-03	3.6909e-03	1.6393e-03	7.2110e-04
			1.0834	1.1433	1.1709	1.1848
ID3-BDF2	-1.8	7.7995e-03	1.8929e-03	4.6855e-04	9.5882e-05	2.2325e-05
			2.0428	2.0143	2.2889	2.1026

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