Modified BDF2 schemes for subdiffusion models with a singular source term

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Outline

Motivation

- 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.

Subdiffusion 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 [1].

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

Since the Riemann-Liouvile fractional derivative and the Caputo fractional derivative can be written in the form

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

which implies that the equivalent form of ($\spadesuit$) can be rewritten as

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

[1] R. Metzler and J. Klafter, *The random walk's guide to anomalous diffusion: a fractional dynamics approach*, Phys. Rep., 339 (2000), pp. 1–77.

Applying the fractional integration operator $J^{1-\alpha}$ to both sides of (♠), we obtain the equivalent form of (♠) as, see [2] [3], namely,

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

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 [4]

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

[2] W. McLean, K. Mustapha, R. Ali, and O. Knio, *Well-posedness of time-fractional advection-diffusion-reaction equations*, Fract. Calc. Appl. Anal., 22 (2019), pp. 918–944.

[3] J. Shen, F. Zeng, and M. Stynes, *Second-order error analysis of the averaged L1 scheme $\overline{L1}$ for time-fractional initial-value and subdiffusion problems*, http://dx.doi.org/10.13140/RG.2.2.24337.35685.

[4] R. Schumer, D.A. Benson, M.M. Meerschaert, and B. Baeumer, *Fractal mobile/immobile solute transport*, Water Resour. Res., 39 (2003), pp. 1–12.

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:

$$ {}^{C}D_t^{\alpha} u(x,t) - Au(x,t) = g(x,t) := t^{\mu} \circ f(x,t) \tag{1} $$

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

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

The well-posedness could be proved using the separation of variables and Mittag–Leffler functions, see [5].

[5] K. Sakamoto and M. Yamamoto, *Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems*, J. Math. Anal. Appl., 382 (2011), pp. 426–447.

For fractional ODEs, one idea is to use starting quadrature weights to correct the fractional integrals [6] (or fractional substantial calculus [7])

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

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 [8].

[6] Ch. Lubich, *Discretized fractional calculus*, SIAM J. Math. Anal., 17 (1986), pp. 704–719.

[7] M.H. Chen and W.H. Deng, *Discretized fractional substantial calculus*, ESAIM: Math. Mod. Numer. Anal., 49 (2015), pp. 373–394.

[8] E. Cuesta, Ch. Lubich, and C. Palencia, *Convolution quadrature time discretization of fractional diffusion-wave equations*, Math. Comput., 75 (2006), pp. 673–696.

- The correction of high-order BDFk convolution quadrature are well developed in [9] [10] when the source term sufficiently smooth in the time variable.
- 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 [11].
- Performing the integral on both sides for (1), e.g, approximate $u(t)$ by $\partial_\tau J^1 u(t)$, a second-order time-stepping schemes are given in [12], where the singular source function is $g(x,t) = t^\mu f(x)$.

How to deal with a more general source term $g(x,t) = t^\mu \circ f(x,t)$?

[9] B. Jin, B.Y. Li, and Z. Zhou, *Correction of high-order BDF convolution quadrature for fractional evolution equations*, SIAM J. Sci. Comput., 39 (2017), pp. A3129–A3152.

[10] J.K. Shi and M.H. Chen, *Correction of high-order BDF convolution quadrature for fractional Feynman-Kac equation with Lévy flight*, J. Sci. Comput., 85 (2020), No. 28.

[11] K. Wang and Z. Zhou, *High-order time stepping schemes for semilinear subdiffusion equations*, SIAM J. Numer. Anal., 58 (2020), pp. 3226–3250.

[12] H. Zhou and W.Y. Tian, *Two time-stepping schemes for sub-diffusion equations with singular source terms*, J. Sci. Comput., 92 (2022), No. 70.

Let $V(t) = u(t) - v$. Then the model (1) can be rewritten as

$$\partial_t^\alpha V(t) - AV(t) = Av + g(t), \quad 0 < t \leq T. \tag{2}$$

Let $G(t) = J^1 g(t)$ and $\mathcal{G}(t) = J^2 g(t)$. We may rewrite (2) as

$$\text{ID1 Method}: \ \partial_t^\alpha V(t) - AV(t) = \partial_t(tAv + G(t)), \quad 0 < t \leq T, \tag{3}$$

$$\text{ID2 Method}: \ \partial_t^\alpha V(t) - AV(t) = \partial_t^2 \left(\frac{t^2}{2} Av + \mathcal{G}(t) \right), \quad 0 < t \leq T. \tag{4}$$

Then IDk-BDF2 method for (3) and (4) are, respectively, designed by

$$\text{ID1} - \text{BDF2 Method}: \quad \partial_\tau^\alpha V^n - AV^n = \partial_\tau(t_n Av + G^n). \tag{5}$$

$$\text{ID2} - \text{BDF2 Method}: \quad \partial_\tau^\alpha V^n - AV^n = \partial_\tau^2 \left(\frac{t_n^2}{2} Av + \mathcal{G}^n \right). \tag{6}$$

Here $\partial_\tau^\alpha \varphi^n := \frac{1}{\tau^\alpha} \sum_{j=0}^n \omega_j \varphi^{n-j}$, and the weights ω_j are given by

$$\delta_\tau^\alpha(\xi) = \frac{1}{\tau^\alpha} \sum_{j=0}^\infty \omega_j \xi^j \quad \text{with} \quad \delta_\tau(\xi) := \frac{1}{\tau} \left(\frac{3}{2} - 2\xi + \frac{1}{2}\xi^2 \right). \tag{7}$$

Taking the Laplace transform in both sides of (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

$$V(t) = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{zt}(z^\alpha - A)^{-1}\left(z^{-1}Av + z\widehat{G}(z)\right)dz \tag{8}$$

with

$$\Gamma_{\theta,\kappa} = \{z \in \mathbb{C} : |z| = \kappa, |\arg z| \le \theta\} \cup \{z \in \mathbb{C} : z = re^{\pm i\theta}, r \ge \kappa\} \tag{9}$$

and $\theta \in (\pi/2, \pi)$, $\kappa > 0$.
Similarly, applying the Laplace transform in both sides of (4), it yields

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

By the inverse Laplace transform, we obtain

$$V(t) = \frac{1}{2\pi i}\int_{\Gamma_{\theta,\kappa}} e^{zt}(z^\alpha - A)^{-1}\left(z^{-1}Av + z^2\widehat{\mathcal{G}}(z)\right)dz. \tag{10}$$

Take $\widetilde{\kappa}(\zeta) = \sum_{n=0}^{\infty} \kappa_n \zeta^n$ to be its generating power series.

Lemma 1

Let δ_τ be given in (7) *and* $\gamma_1(\xi) = \frac{\xi}{(1-\xi)^2}$, $G(t) = J^1 g(t)$. *Then the discrete solution of* (5) *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 $\Gamma^\tau_{\theta,\kappa} = \{z \in \Gamma_{\theta,\kappa} : |\Im z| \leq \pi/\tau\}$.

Lemma 2

Let δ_τ be given in (7) *and* $\gamma_2(\xi) = \frac{\xi+\xi^2}{(1-\xi)^3}$, $\mathcal{G}(t) = J^2 g(t)$. *Then the discrete solution of* (6) *is represented by*

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

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

Let $V(t_n)$ and V^n be the solutions of (3) and (5), respectively. Let $v = 0$ and $G(t) := \frac{t^l}{l!} g^{(l-1)}(0)$ with $l = 0, 1, 2$. Then

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

Lemma 4

Let $V(t_n)$ and V^n be the solutions of (3) *and* (5)*, 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*

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

Theorem 5 (ID1-BDF2)

Let $V(t_n)$ and V^n be the solutions of (3) *and* (5)*, respectively. Let $v \in L^2(\Omega)$, $g \in C^1([0,T]; L^2(\Omega))$ and $\int_0^t (t-s)^{\alpha-1}\left\|g''(s)\right\| ds < \infty$. Then the following error estimate holds for any $t_n > 0$:*

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

Theorem 6 (ID2-BDF2)

Let $V(t_n)$ and V^n be the solutions of (4) and (6), 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 $t_n > 0$:

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

Form Theorem 5 and Theorem 6, 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 $t^\mu q(x)$.

In the section, we first consider low regularity source term $g(x,t) = t^{\mu}q(x)$ with $\mu > 0$ for subdiffusion (3). We introduce the polylogarithm function or Bose-Einstein integral

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

Lemma 7

[a] *Let $|z\tau| \leq \frac{\pi}{\sin\theta}$ and $\theta > \pi/2$ be close to $\pi/2$, and $p \neq 1, 2, \ldots$. The series*

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

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

[a] B. Jin, R. Lazarov, and Z. Zhou, *An analysis of the L1 scheme for the subdiffusion equation with nonsmooth data*, IMA J. Numer. Anal., 36 (2016), pp. 197–221.

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 (8), we have

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

From Lemma 1, the discrete solution for the subdiffusion (5) is

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

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

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

Lemma 8

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*

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

Proof.

Using the definitions of $\widehat{G}(z)$ and $\widetilde{G}(e^{-z\tau})$ and Lemma 7 with $p = -\mu - 1$, we have

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

Theorem 9 (ID1-BDF2)

Let $V(t_n)$ and V^n be the solutions of (3) and (5), respectively. Let $v \in L^2(\Omega)$ and $g(x,t) = t^{\mu}q(x)$, $\mu > 0$, $q(x) \in L^2(\Omega)$. Then

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

Lemma 10

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

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

Theorem 11 (ID2-BDF2)

Let $V(t_n)$ and V^n be the solutions of (4) and (6), 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

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

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

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

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 12

Let $V(t_n)$ and V^n be the solutions of (3) and (5), 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

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

Theorem 13 (ID1-BDF2)

Let $V(t_n)$ and V^n be the solutions of (3) and (5), 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

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

Proof.

According to Theorem 9, Lemma 12, and similar treatment of the initial data v in Theorem 5, the desired result is obtained. □

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 $h(t) = t^\mu (t * f''(t))$ 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

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

Moreover, there exists

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

Thus one has

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

Lemma 14

Let $V(t_n)$ and V^n be the solutions of (3) and (5), 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

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

Theorem 15 (ID1-BDF2)

Let $V(t_n)$ and V^n be the solutions of (3) and (5), 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

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

Convergence analysis: product source function $t^\mu f(t)$, $\mu > -1$. Let $\mathcal{G}(t) = J^2 g(t)$ and $f(t) = f(0) + tf'(0) + t * f''(t)$. Then we have

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

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

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

which implies

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

since

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

Thus we get

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

Lemma 16

Let $V(t_n)$ and V^n be the solutions of (4) and (6), respectively. Let $v = 0$, $\mathcal{G}(t) = t * [t^{\mu}(t * f''(t))]$ with $-\alpha \leq \mu < 0$ and $f \in C^1([0,T]; L^2(\Omega))$, $\int_0^t s^{\frac{\mu-1}{2}} \|f''(s)\| \, ds < \infty$, $\int_0^t (t-s)^{\alpha-1} s^{\mu} \|f''(s)\| \, ds < \infty$. Then

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

Theorem 17 (ID2-BDF2)

Let $V(t_n)$ and V^n be the solutions of (4) and (6), respectively. Let $v \in L^2(\Omega)$, $g(t) = t^{\mu} f(t)$ with $-\alpha \leq \mu < 0$ and $f \in C^1([0,T]; L^2(\Omega))$, $\int_0^t s^{\frac{\mu-1}{2}} \|f''(s)\| \, ds < \infty$, $\int_0^t (t-s)^{\alpha-1} s^{\mu} \|f''(s)\| \, ds < \infty$. Then

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

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

$$\text{BDF2 Method}: \quad \partial_\tau^\alpha V^n - AV^n = Av + g^n. \tag{11}$$

$$\text{Corr}-\text{BDF2 Method}: \quad \partial_\tau^\alpha V^n - AV^n = \frac{3}{2}Av + \frac{1}{2}g^0 + g^n. \tag{12}$$

Example 18

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

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

Here $J^k g(x,t) = t^{k-1} * g(x,t)$, $k = 1, 2$ are calculated by JacobiGL Algorithm [13], which is generating the nodes and weights of Gauss-Labatto integral with the weighting function such as $(1-t)^\mu$ or $(1+t)^\mu$.

[13] J.S. Hesthaven and T. Warburton, *Nodal Discontinuous Galerkin Methods: Algorithms, Analysis, and Application*, Springer, 2007.

Table 1: The discrete L^2-norm $||u^N - u^{2N}||$ and convergent order of schemes (11), (12) and (5), (6) 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

Table 2: The discrete L^2-norm $||u^N - u^{2N}||$ and convergent order of schemes (5) and (6) 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 3: The discrete L^2-norm $||u^N - u^{2N}||$ and convergent order of schemes (11) and (5) 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

For subdiffusion PDEs model (1), it is natural appearing the low regularity/singular term such as

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

In this case, many popular time stepping schemes, including the correction of high-order BDF methods may lose their high-order accuracy, see [14]. The correction BDF2 methods recovers superlinear 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 1 and 2. Tables 3 shows that ID1-BDF2 recovers second order convergence and this is in agreement with the order of the convergence for $t^{\mu} * f(x,t)$, $\mu > -1$.

[14] K. Wang and Z. Zhou, *High-order time stepping schemes for semilinear subdiffusion equations*, SIAM J. Numer. Anal., 58 (2020), pp. 3226–3250.

For Hadamard's finite-Part integral [15]

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

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 4.

Table 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

[15] K. Diethelm, *The Analysis of Fractional Differential Equations*, Springer, 2010.

It is easy to extend the higher order schemes, e.g., ID2-BDF3, ID3-BDF4, see Table 5.

Table 5: The discrete maximum-norm $||u^N - u^{2N}||$ and convergent order of ID2-BDF3 and ID3-BDF4 scheme for Example 18 with $g(x,t) = 0$.

Scheme	α	$N = 40$	$N = 80$	$N = 160$	$N = 320$	$N = 640$
ID2-BDF3	0.3	2.2976e-07	2.7210e-08	3.3127e-09	4.0871e-10	5.0758e-11
			3.0779	3.0380	3.0188	3.0093
	0.7	7.0505e-07	8.2623e-08	1.0008e-08	1.2317e-09	1.5278e-10
			3.0930	3.0453	3.0224	3.0111
ID3-BDF4	0.3	2.5000e-08	1.4195e-09	8.4663e-11	5.1885e-12	3.9823e-13
			4.1384	4.0675	4.0283	3.7036
	0.7	8.5711e-08	4.8005e-09	2.8439e-10	1.7327e-11	1.14674e-12
			4.1582	4.0772	4.0367	3.9174

This talk is based on [16].

[16] M.H. Chen, J.K. Shi, Z. Zhou, *Modified BDF2 schemes for subdiffusion models with a singular source term*, arXiv:2207.08447.

Thanks for your attention!