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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 an m-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. The proposed approach is applicable for stochastic subdiffusion equation.

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

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 [22, 23]. 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 [23, Eq. (88)]

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

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 [26, 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

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

with the Caputo fractional derivative

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

Applying the fractional integration operator $J^{1-\alpha}$ to both sides of (♠), we obtain the equivalent form of (♠) as, see [21, Eq. (1.6)] or [31, Eq. (2.3)], namely,

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

As another example, the fractal mobile/immobile models for solute transport associated with power law decay PDF describing random waiting times in the immobile zone, lead to the following models [29, 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 the aforementioned PDE models (♠)-(♢) might be nonsmooth in the time variable. In this paper, we consider the subdiffusion model with weakly singular source term:

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

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

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

The well-posedness could be proved using the separation of variables and Mittag–Leffler functions, see e.g. [27, 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 [11, 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 [35], also see Table 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) (e.g., $f = 0$) does not imply the smoothness of the solution u which has an initial layer at $t \to 0^+$ (i.e., unbounded near $t = 0$) [26, 27, 33]. 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, 15, 17, 20, 25, 24, 33]. See also spectral method with specially designed basis functions [4, 8, 38]. The second type is based on correction of high-order BDFk or L_k approximation, and then the desired high-order convergence rates can be restored even for nonsmooth initial data [5, 19, 18, 9, 11, 35]. For fractional ODEs, one idea is to use starting quadrature weights to correct the fractional integrals [18] (or fractional substantial calculus [1])

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