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Numerical solution of space fractional diffusion equation by the method of lines and splines

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ABSTRACT

This paper is devoted to the application of the method of lines to solve one-dimensional diffusion equation where the classical (integer) second derivative is replaced by a fractional derivative of the Caputo type of order α less than 2 as the space derivative. A system of initial value problems approximates the solution of the fractional diffusion equation with spline approximation of the Caputo derivative. The result is a numerical approach of order $\mathcal{O}(\Delta x^2 + \Delta t^m)$, where Δx and Δt denote spatial and temporal step-sizes, and $1 \leq m \leq 5$ is an integer which is set by an ODE integrator that we used. The convergence and numerical stability of the method are considered, and numerical tests to investigate the efficiency and feasibility of the scheme are provided.

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1. Introduction

Fractional partial differential equations (FPDEs), as generalizations of the classical integer order partial differential equations, appear in many applications of the applied sciences to model problems in fluid flow, finance, phase transitions, stratified materials and anomalous diffusions [1–5]. Numerical schemes for FPDEs are relatively sparse, and the majority of the publications are based on finite difference methods and finite element methods (see e.g., [6–13]).

Fractional order diffusion equations are generalizations of classical diffusion equations. They have been used in a broad variety of applications in fluid flow, finance, seeds dispersion engineering, description of a fractional random walk, biological and physical processes where anomalous diffusion occurs [14–20].

Fractional space derivatives are used to formulate anomalous dispersion models, where a particle plume spreads at a rate that is different than the classical Brownian motion model [21]. Here, we are concerned with a fractional diffusion model with a spatial derivative of fractional order $1 < \alpha \leq 2$.

Consider the one-dimensional space fractional diffusion equation (SFDE) with source term of the form

$$\frac{\partial u(x,t)}{\partial t} = d(x,t)\,\frac{\partial^{\alpha} u(x,t)}{\partial x^{\alpha}} + p\big(x,t,u(x,t)\big), \qquad (x,t) \in \Omega, \tag{1}$$

where $1 < \alpha \leq 2$, $\Omega = \{(x,t) : a < x < b,\ t > 0\}$, and continuous function $d(x, t) > 0$ denotes the diffusion coefficient (or diffusivity). The forcing function $p(x, t, u(x, t))$ which is assumed to be continuous and satisfies the Lipschitz condition with respect to third argument, can be used to represent sources and sinks, and may given as nonlinear function in $u(x, t)$. The

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initial condition of the SFDE (1) is given as

$$u(x,0) = \phi(x), \qquad a < x < b, \tag{2}$$

and Robin boundary conditions (BCs) are

$$c_1(t)\,u(a,t) + c_2(t)\,\frac{\partial u(a,t)}{\partial x} = h_1(t), \tag{3-1}$$

$$c_3(t)\,u(b,t) + c_4(t)\,\frac{\partial u(b,t)}{\partial x} = h_2(t), \tag{3-2}$$

where $c_1(t)$, $c_2(t)$ and $c_3(t)$, $c_4(t)$ do not vanish simultaneously for $t > 0$. This means that, for example, if $c_2(t) = 0$ for some $t > 0$, we must have $c_1(t) \neq 0$ for all $t > 0$. Note that if $c_2(t) = c_4(t) = 0$, we have Dirichlet BCs, and if $c_1(t) = c_3(t) = 0$, we have Neumann BCs. Although in most practical applications $\{c_i(t)\}_{i=1}^{4}$ are given as constants, but here we consider the general case of variation with t.

Throughout this paper, $\frac{\partial^\alpha u(x,t)}{\partial x^\alpha}$ denotes the fractional derivative of order $1 < \alpha \le 2$ in the Caputo sense, defined by [22,23]:

$$\frac{\partial^\alpha u(x,t)}{\partial x^\alpha} = \frac{1}{\Gamma(2-\alpha)} \int_a^x (x-s)^{1-\alpha}\, \frac{\partial^2 u(s,t)}{\partial s^2}\, \mathrm{d}s. \tag{3}$$

The existence and uniqueness of the solution for SFDE (1) subject to its initial and boundary conditions, have been investigated by Baeumer et al. [24]. They have also shown that the solution is non-negative when the initial condition is non-negative. We aslo assume that this fractional diffusion equation has a sufficiently smooth solution under its initial and boundary conditions.

Numerical approaches to solve SFDEs with Dirichlet BCs have been gaining increased attention in the literature. In the case $p\big(x,t,u(x,t)\big) = p(x,t)$, Khader [25] used a Chebyshev collocation method to discretize Eq. (1) to get a linear system of ordinary differential equations (ODEs) and used finite differences (FDs) to solve the resulting ODE system. Zhu [26] studied SFDEs with fractional Fellers operator. Saadatmandi and Dehghan [27] introduced approximation techniques based on the shifted Legendre–tau (SLT) scheme. Ren et al. [28] presented a method based on the shifted Chebyshev-tau, and using the operational matrix of the fractional derivative, reduced the problem to a set of linear algebraic equations. Sousa [29] presented an implicit numerical method which used a spline approximation to approximate the fractional derivative.

For nonlinear source term, numerical computations without any theoretical discussions are carried out by Lynch et al. [30]. Choi et al. [31] considered the backward Euler FD method to obtain numerical solutions for the fractional differential dispersion equations with nonlinear forcing terms and obtained an error estimate of order $\mathcal{O}(\Delta x + \Delta t)$ in the discrete L_2 norm, where Δx and Δt denote spatial and temporal step-sizes, respectively.

In this paper, the Sousa approach [29] is extended from Dirichlet to Robin BCs, and by application of the method of lines (MOL) extended to solve nonlinear SFDEs of the type (1). The error analysis established that our method is stable and convergent of $\mathcal{O}(\Delta x^2 + \Delta t^m)$ where $1 \le m \le 5$ is an integer. The efficiency of the current method is demonstrated through a comparison with a method reported in [27] and the method originally reported by Sousa [29]. Further, the present method is verified by application to some test problems with exact solutions.

The basic algorithm was reported by Sousa [29] in which the Caputo derivative is approximated by linear splines in a numerical quadrature for the defining integral (see below for details). Rather than using the Crank–Nicolson method for the time integration as in [29], the approximating system of initial value problems is integrated by the library ODE integrator in R[1], `lsodes`, that is variable step and variable order, with the order starting at one initially (the implicit Euler method, $m = 1$) and extending to a fifth order backward differentiation formula (BDF) ($m = 5$) as the solution evolves.

The outline of the paper is as follows: Section 2 is devoted to a brief survey on BDF methods. In Section 3, we describe the numerical method to approximating the solution of Eq. (1). We have presented the error analysis of the current method in Section 4. In Section 5, numerical results are reported to demonstrate the efficiency and convergence of the scheme. Finally we end the paper with some concluding remarks in Section 6.

2. A survey on BDF methods

The BDF methods are an important class of very effective numerical schemes to solve stiff initial value problems, firstly introduced by Curtiss and Hirschfelder [32]. Enright et al. [33] established that the BDF methods are unrivaled for solving stiff problems whose eigenvalues are not close to the imaginary axis.

To start the introduction of the BDF methods, consider the following system of initial value problems (IVPs)

$$\vec{y}'(t) = \vec{f}(t, \vec{y}(t)), \qquad \vec{y}(0) = \vec{y}_0, \tag{4}$$

where the unknown function $\vec{y}(t)$ is assumed to be sufficiently smooth and the right hand side function $\vec{f}$ is continuous and satisfies a Lipschitz condition for some constant $L > 0$.

[1] R is a quality open source scientific programming system that can be easily downloaded from the Internet (http://www.R-project.org/).