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Numerical solution of time fractional diffusion systems

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ABSTRACT

In this paper a general class of diffusion problem is considered, where the standard time derivative is replaced by a fractional one. For the numerical solution, a mixed method is proposed, which consists of a finite difference scheme through space and a spectral collocation method through time. The spectral method considerably reduces the computational cost with respect to step-by-step methods to discretize the fractional derivative. Some classes of spectral bases are considered, which exhibit different convergence rates and some numerical results based on time diffusion reaction diffusion equations are given.

1. Introduction

Although fractional calculus dates back to the XIX century, only in the last 50–60 years has growing interest been paid to this subject in modelling applications. The time fractional derivative ${}_0D_t^{\alpha}y(t)$ depends on the past history of the function $y(t)$, and so time fractional differential systems are naturally suitable to describe evolutionary processes with memory when $0<\alpha\leq 1$. For values $1<\alpha\leq 2$ the phenomena that are modelled have wave like properties – see [13]. Fractional models are increasingly used in many modelling situations including viscoelastic materials in mechanics [30,42], anomalous diffusion in transport dynamics of complex systems [25,33], soft tissues such as mitral valve in the human heart [40], some biological processes in rheology [12], the kinetics of complex systems in spatially crowded domains (compare [1] and references therein contained), the spread of HIV infection of CD4+ T-cells [11], Brownian motion [31,34]. A number of applications modelled by time-fractional differential equations can be found in [21] and in the references therein. In many cases, the derivative index α belongs to the interval $(0,1)$, like in [1,11–13,40,41].

One important application area where both time and space fractional models are becoming important is in the field of water diffusion magnetic resonance imaging. Conventional MRI studies are based on the assumption of Gaussian diffusion, but biological tissues are structurally heterogeneous and under large diffusion weighting gradients the acquired signal has a heavy tail which is characteristic of anomalous diffusion [18] and hence fractional diffusion models are relevant. Anomalous diffusion MRI studies have been conducted in the brain [19], cardiac tissue [6], liver [3] and cartilage [37]. Specifically time

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fractional diffusion MRI models have been developed in [29,32,17], while fractional diffusion models of cardiac electrical propagation have been considered in [5,8].

In this paper we consider a time-fractional reaction diffusion problem

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2}{\partial x^2}u(x,t) + f(t,x), \qquad (x,t) \in [0,X] \times [0,T], \tag{1.1}$$

subject to boundary conditions (such as Neumann or Dirichlet boundary conditions) as well as to suitable initial conditions. Here $u : [0,T] \times [0,X] \to \mathbb{R}$, $f : [0,T] \times [0,X] \to \mathbb{R}$. If $0 < \alpha \leq 1$ initial conditions are of the type $u(x,0) = u_0(x)$, if $1 < \alpha \leq 2$ initial conditions are of the type $u(x,0) = u_0(x)$, $u_t(x,0) = u_{t,0}(x)$ (compare [2,21] and references therein). In the following we restrict our attention to the case $0 < \alpha < 1$. Some results of existence and uniqueness of solution can be found in [27,28], where the analytical solution is also expressed in form of Fourier series. We adopt Caputo's definition of fractional derivative:

$$\frac{\partial^\alpha y(t)}{\partial t^\alpha} = {}_0D_t^\alpha y(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{y^{(n)}(\tau)}{(t-\tau)^{\alpha+1-n}} d\tau, \quad n-1 < \alpha < n, \; n \in \mathbb{N}.$$

Some fundamental notions on fractional calculus may be found in [35].

One of the features of time fractional models is that they are examples of non-local models and as the solution depends on all its past history, numerical step-by-step methods are computationally expensive. On the other hand, it is well known that spectral methods can avoid the discretization of the 'heavy tail' and are exponentially convergent [23,26,41,45,46] and so are suitable for non-local problems avoiding the difficulty of using time discretization techniques that need to use all, or most, of the history. This motivates us to use a numerical scheme consisting of a spectral method through time, on a suitable basis of functions, and a finite-difference method through space, whose coefficients are adapted according to the qualitative behavior of the solution.

The paper is organized as follows. In Section 2 we introduce a mixed spectral collocation method, applied to the semi-discrete problem generated by a finite difference scheme through space. Section 3 deals with the computation of matrix **D** and vector **d**, which is a crucial part of the overall method. Section 4 is devoted to the choice of the bases of functions of the spectral method and of the collocation points. Some numerical experiments are illustrated in Section 5. Finally, we give some concluding remarks.

2. The method

We consider in a first analysis the time-fractional diffusion problem (1.1) subject to Neumann boundary conditions and initial conditions:

$$\frac{du(0,t)}{dx} = \frac{du(X,t)}{dx} = 0, t \in [0,T], \quad u(x,0) = u_0(x), x \in [0,X]. \tag{2.1}$$

2.1. Semi-discretization through space

The first step to solve the problem (1.1), (2.1) consists of applying a finite-difference scheme to discretize the spatial derivative. We use a space discretization which is suitable to treat both Neumann and Dirichlet condition. We introduce a uniform mesh on $[0,X]$, given by:

$$x_0 = 0 < x_1 < \cdots < x_M, \quad x_m = m\Delta x, \quad \Delta x = X/M.$$

To approximate the spatial derivative in (1.1), in the internal points, we adopt this centered finite difference scheme:

$$\frac{\partial^2 u(x_i,t)}{\partial x^2} = \frac{a_2 u(x_{i-1},t) + a_1 u(x_i,t) + a_0 u(x_{i+1},t)}{(\Delta x)^2} + \frac{\partial^4 u(\xi,t)}{\partial x^4}\frac{(\Delta x)^2}{12}, \tag{2.2}$$

$\xi \in [x_{i-1}, x_{i+1}]$, assuming that u is sufficiently smooth.

In the case of the classical centered finite difference scheme, we have $a_0 = a_2 = -1$ and $a_1 = 2$. Alternatively, if the solution has an oscillatory behavior with respect to the spatial variable, and an estimate of the frequency is available, we may apply the exponentially-fitted centered finite difference scheme introduced in [9,10] (compare also [7]). We refer to [9] for the exact expression of coefficients a_0, a_1 and a_2 in this case. An extensive monograph on the exponential fitting theory is [20].

At the boundary, we consider two different second order approximations of the Neumann condition: the centered difference approximation

$$u_x(x,t) = \frac{u(x+\Delta x,t) - u(x-\Delta x,t)}{2\Delta x} + \frac{(\Delta x)^2}{6} u_{xx}(x,t) + O((\Delta x)^4) \tag{2.3}$$