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# A fourth-order extrapolated compact difference method for time-fractional convection-reaction-diffusion equations with spatially variable coefficients<sup>‡</sup>

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#### ABSTRACT

This paper is concerned with numerical methods for a class of time-fractional convectionreaction-diffusion equations. The convection and reaction coefficients of the equation may be spatially variable. Based on the weighted and shifted Grünwald–Letnikov formula for the time-fractional derivative and a compact finite difference approximation for the spatial derivative, we establish an unconditionally stable compact difference method. The local truncation error and the solvability of the resulting scheme are discussed in detail. The stability of the method and its convergence of third-order in time and fourth-order in space are rigorously proved by the discrete energy method. Combining this method with a Richardson extrapolation, we present an extrapolated compact difference method which is fourth-order accurate in both time and space. A rigorous proof for the convergence of the extrapolation method is given. Numerical results confirm our theoretical analysis, and demonstrate the accuracy of the compact difference method and the effectiveness of the extrapolated compact difference method.

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#### 1. Introduction

Fractional differential equations have numerous effective applications to various areas of science and engineering (see [4–6,24,25,28,37,38,40–42]). It has been proved that these equations are more appropriate for the description of memorial and hereditary properties of various materials and processes than classical differential equations of integer-order. Qualitative analysis of these equations can be found in the review article [40] and monograph [42]. We also see [1,22,39,44,50] for some more recent theoretical developments.

Time-fractional diffusion equations are often used to describe the transport dynamics in various complex systems where Gaussian statistics are no longer followed and the Fick second law fails to describe the related transport behaviors. One simple form of this kind of equations is taken as

$${}^{C}_{0}\mathcal{D}^{\alpha}_{t}\nu(x,t) = d\frac{\partial^{2}\nu}{\partial x^{2}}(x,t) + f(x,t), \quad (x,t) \in (0,L) \times (0,T),$$

$$(1.1)$$

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where the term  ${}^{C}_{0}\mathcal{D}^{\alpha}_{t}v(x,t)$  represents the Caputo time-fractional derivative of order  $\alpha$ , which is defined by

$${}^{C}_{0}\mathcal{D}^{\alpha}_{t}\nu(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{\partial \nu}{\partial s}(x,s)(t-s)^{-\alpha} \mathrm{d}s, \quad 0 < \alpha < 1.$$
(1.2)

Another form is given in the Riemann–Liouville time-fractional derivative sense and the corresponding equation is equivalent to the equation (1.1) under some regularity assumption for v(x, t) in time (see [19,53]).

For a general source term f, it is usually difficult to obtain analytical solutions for the fractional differential equations in the form (1.1). Various numerical methods have been developed to obtain their approximate solutions (see [8–10,12,20,23,29,31,33–36,51,52,54,56–58]). Unlike the classical case, the Caputo time-fractional derivative (1.2) is nonlocal and has the character of history dependence and universal mutuality. This implies that, we require solution information on all the previous time levels for computing the solution on the current time level, and thus the computations are rather time-consuming even in one-dimensional case. For this reason, it is very important to construct a stable numerical approximation scheme of high-order. In order to obtain a high-order space approximation, a commonly used difference approach is to adopt the compact difference scheme (see [8,20,54]). This method achieves the fourth-order accuracy while retaining the tridiagonal feature of a second-order method. However, it is difficult to get a high-order time approximation due to the singularity of the time-fractional derivative.

Traditionally, the *L*1 formula is often used to approximate the Caputo time-fractional derivative (1.2) (see [2,8,15,20,34,41,45,54]). However, the corresponding difference scheme has been proved to have only the temporal accuracy of order  $2 - \alpha$  which is less than two (see [20,34,45]). In [21], a modified *L*1 formula (called the *L*1 – 2 formula) was presented. This formula improves the numerical accuracy of the *L*1 formula, but the strict convergence analysis for the corresponding difference scheme has not been available. In order to get a provable convergence, another modified *L*1 formula (called the *L*2 –  $1_{\sigma}$  formula) was given in [3], where it was proved that the corresponding difference scheme possesses the second-order temporal convergence. More recently in [7,32], a series of new high-order approximations to the Caputo time-fractional derivative (1.2) were derived. These approximations extend the *L*1 – 2 formula and have the numerical accuracy of order  $r - \alpha$ , where  $r \ge 4$  is a positive integer. Also discussed in [7,32] is the applications of the derived approximations to a time-fractional advection-diffusion equation with constant coefficients. A high-order finite difference scheme using the standard second-order central difference approximation for the spatial derivative was proposed there and the "practical numerical stability" of the scheme was then proved by the Fourier method.

Another way to design high-order approximations to the fractional derivative is to utilize the Grünwald–Letnikov formula or Lubich formula. These formulae are often used to handle the Riemann–Liouville fractional derivative (see [18,19,30,47,49,55]). Based on the Grünwald–Letnikov formula and the equivalence of Riemann–Liouville and Caputo derivatives under some regularity assumptions, the authors of [26] derived a third-order approximation formula for the Caputo time-fractional derivative (1.2). Then they constructed the corresponding compact difference scheme (called the *GL*<sub>3</sub> scheme) in [26] for the time-fractional diffusion equation (1.1) and in [27] for its two-dimensional case. In order to attain third-order temporal convergence of the *GL*<sub>3</sub> scheme, a transformation of the time-fractional diffusion equation (1.1) into its equivalent integro-differential form is required in [26] for the discretization on the first time level. As a result, the Riemann–Liouville fractional integral  $_0 D_t^{-\alpha} f(x, t)$  of the source term f(x, t) must be found in advance before applying the *GL*<sub>3</sub> scheme, where

$${}_{0}\mathcal{D}_{t}^{-\alpha}f(x,t) = \frac{1}{\Gamma(\alpha)} \int_{0}^{t} f(x,s)(t-s)^{\alpha-1} \mathrm{d}s.$$
(1.3)

One aim of this paper is to present a new technique for the discretization on the first time level. This new technique avoids computing the fractional integral  ${}_{0}\mathcal{D}_{t}^{-\alpha}f(x,t)$  so that the resulting scheme appears more simple in computation, but still maintains third-order temporal convergence. In addition, we make further investigations on the truncation error of the Grünwald–Letnikov formula to obtain two explicit asymptotic error expansions. Based on these asymptotic error expansions, we establish an extrapolated compact difference method to further improve the temporal accuracy of the computed solution.

In order to enlarge the applications of our method, we extend the constant coefficient equation (1.1) to a class of more general time-fractional convection-reaction-diffusion equations with variable coefficients. The class of equations under consideration with its boundary and initial conditions is given by

$$\begin{cases} {}^{C}_{0}\mathcal{D}^{\alpha}_{t}v(x,t) = d\frac{\partial^{2}v}{\partial x^{2}}(x,t) - p_{1}(x)\frac{\partial v}{\partial x}(x,t) + p_{2}(x)v(x,t) + f(x,t), & (x,t) \in (0,L) \times (0,T), \\ v(0,t) = \phi_{0}(t), & v(L,t) = \phi_{L}(t), & t \in (0,T], \\ v(x,0) = \varphi(x), & x \in [0,L], \end{cases}$$
(1.4)

where *d* is a known positive constant. Throughout the paper, we shall assume that the given functions  $p_1(x)$ ,  $p_2(x)$ , f(x, t),  $\phi_0(t)$ ,  $\phi_L(t)$  and  $\varphi(x)$  in (1.4) are smooth enough and the solution to the problem (1.4) has the necessary regularity (see the assumptions in Theorem 3.1 and Lemma 5.3).

There is relatively little discussion on numerical methods for the variable coefficient problem (1.4). A class of finite difference methods with the temporal accuracy of order  $2 - \alpha$  at most and the second-order spatial accuracy was developed in [11]. The works in [13,14] were devoted to a combined compact finite difference method and a compact exponential finite difference method. But, the stability and convergence analysis given there was still limited to the special case of constant coefficients, and the numerical accuracy of the method for the variable coefficient case was exhibited only through a variety

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