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Jacobi Spectral Collocation Method for the Time Variable-Order Fractional Mobile-Immobile Advection-Dispersion Solute Transport Model

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Abstract. An efficient high order numerical method is presented to solve the mobile-immobile advection-dispersion model with the Coimbra time variable-order fractional derivative, which is used to simulate solute transport in watershed catchments and rivers. On establishing an efficient recursive algorithm based on the properties of Jacobi polynomials to approximate the Coimbra variable-order fractional derivative operator, we use spectral collocation method with both temporal and spatial discretisation to solve the time variable-order fractional mobile-immobile advection-dispersion model. Numerical examples then illustrate the effectiveness and high order convergence of our approach.

AMS subject classifications: 26A33, 65M70, 15A99, 39A70

Key words: Coimbra variable-order fractional derivative, Jacobi polynomials, spectral collocation method, Mobile-immobile advection-dispersion model.

1. Introduction

Fractional calculus involves fractional integral or fractional derivative operators that extend the notions of integer-order differentiation and integration to any real or complex-order [1–4]. There are many scientific and engineering applications — e.g. to model electrochemical processes [5], porous or fractured media [6], viscoelastic materials [7, 8] and aspects of bioengineering [9].

It is well known that fractional derivative operators are nonlocal with weak singularity, so become more complicated for theoretical analysis and numerical simulation. In recent years, considerable effort has been devoted to the numerical solution of problems involving fractional integral and derivative operators, including finite difference methods [10–13], finite element methods [14–16] and spectral methods [17–19]. Jacobi polynomials are often used to solve fractional differential equations (FDE) when spectral methods are adopted,

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given the intrinsically singular kernels of the fractional operators that induce singular solutions or data. Thus even if an FDE has a smooth solution, the source term might have singular behaviour, or vice versa. Furthermore, the singularity can be linked to the Jacobi weight function. For example, an FDE in 1D on the standard interval $[-1,1]$ may involve a singular factor $(1+x)^{-\mu}$ at $x=-1$ for the left fractional derivative and $(1-x)^{-\mu}$ at $x=1$ for the right fractional derivative, where μ denotes the order of the fractional derivative. Jacobi polynomials have been widely used to approximate functions with such singularities in spectral methods.

Evolution equations involving fractional derivatives have proven to be more accurate for describing anomalous diffusion and transport dynamics in complex systems. It has also been found that many physical processes appear to exhibit fractional order behaviour varying in time or space, so variable-order (VO) fractional calculus arises in corresponding complex dynamical problems. Pioneering work on VO fractional operators was undertaken by Samko & Ross [21], who introduced VO Riemann-Liouville fractional integration and differentiation. Subsequently, VO fractional operators have been invoked in mathematical modelling in various fields, including viscoelasticity [22] and anomalous diffusion [23]. Various definitions of VO fractional operators have been suggested [20,22,24,25], each preferred for different reasons. Quite recently, Ramirez & Coimbra [25] compared nine definitions of VO fractional derivative (integral) operators based on a few criteria: "(a) the VO operator must be able to return all intermediate values between 0 and 1 that correspond to the argument of the order of differentiation; (b) the VO operator must be effectively evaluated numerically; and (c) all derivatives of a true constant (a function that is constant from $-\infty$ to $+\infty$) must be zero". They concluded that only the VO fractional derivative defined in Ref. [22] satisfied all these criteria when modelling dynamic systems.

Since the kernel of VO operators have a variable exponent, analytical solutions to VO fractional differential equations (VOFDE) are more difficult to obtain and research on the solution of VOFDEs is relatively new, and the numerical approximation of VOFDEs is consequently also at an early stage of development. Liu and collaborators have studied the stability and convergence of diverse FD schemes for a class of VOFDE, including the VO nonlinear fractional diffusion equation [26], the VO space fractional advection-diffusion equation with a nonlinear source term [27], and the time variable fractional order mobile-immobile advection-dispersion model [28]. Sun *et al.* [29] applied three FD schemes for a series of VO time fractional diffusion equations, and Zhao *et al.* [30] derived two second-order approximation formulas for the VO fractional time derivatives involved in anomalous diffusion and wave propagation. Operational matrix methods to discretise the VO cable equation have also been proposed [31,32].

Compared to such developments on FD schemes for VOFDE, global and high order spectral methods have received little attention. However, VO fractional operators with weak singularities previously seen in classical fractional operators are also nonlocal, so spectral methods using Jacobi polynomials seems a natural choice to develop global high order numerical schemes for solving VOFDEs numerically. Recently, Zayernouri *et al.* [33] proposed fractional spectral collocation methods for linear and nonlinear variable order FPDE that employ fractional basis functions they called "Jacobi polyfractonomials", and