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Original articles

A Green's function approach for the numerical solution of a class of fractional reaction–diffusion equations

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Highlights

- Numerical solutions of fractional RD systems are given using Green's function formulations.
- The scheme proposed exhibit global approximation orders of $O(h^{\alpha})$.
- Proposed scheme exhibit better numerical approximation than traditional schemes.

Abstract

Reaction–diffusion equations with spatial fractional derivatives are increasingly used in various science and engineering fields to describe spatial patterns arising from the interaction of chemical or biochemical reactions and anomalous diffusive transport mechanisms. Most numerical schemes to solve fractional reaction–diffusion equations use finite difference schemes based on the Grünwald–Letnikov formula. This work introduces a new systematic approach based on Green's function formulations to obtain numerical schemes for fractional reaction–diffusion equations. The idea is to pose an integral formulation of the equation in terms of the underlying Green's function of the fractional operator to subsequently use numerical quadrature to obtain a set of ordinary differential equations. To illustrate the numerical accuracy of the method, dynamic and steady-state situations are considered and compared with analytical and numerical solutions via Grünwald finite differences schemes. Numerical simulations show that the scheme proposed improves the performance and convergence of traditional finite differences schemes based on Grünwald formula.
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1. Introduction

Reaction–diffusion systems have been used in various science and engineering fields. However, recent research indicates that the classical diffusion equation is inadequate to model many real situations. For example, in processes

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where the particles spread at a faster rate than that predicted by Fickian diffusion and can present asymmetry. This phenomenon is commonly known as anomalous diffusion [23,27]. Fractional reaction–diffusion equations can describe a large number of physical processes controlled by anomalous diffusion. Some example include, solute transport [31], transport in plasma turbulence [7], in the pattern formation [13,12], transport at the Earth surface [30], diffusion through porous materials [3,34]. Lenzi et al. [18] showed that the anomalous diffusion is a suitable framework for modeling transport in catalytic particles. Recently, Zheng et al. [38] considered fractal theory for modeling diffusion in porous media, finding good agreement between experimental data and theoretical predictions. On the other hand, Das [6] computed approximate analytical solutions for fractional diffusion equations that can be used in the modeling of reaction–diffusion in catalytic systems. Liu et al. [21] used a fractional differential equation to describe anomalous diffusion in a mobile/immobile transport model. Friess et al. [11] showed that non-Fickian diffusion phenomenon should be considered for describing transport of some alcohol vapors in teflon material.

Different numerical methods have been used to solve both linear and nonlinear fractional reaction–diffusion equations such as, standard discretization of the fractional-in-space operator [16], Fourier methods [4], homotopy methods [17], finite element [37] and Grünwald fractional difference (GrFD). Due to its simplicity of computational implementation, the latter is the most commonly used [22,8,25,5]. However, it is well-known that the discretization of fractional derivatives by means of GrFD is of first-order accurate $O(h)$ and it may lead to instabilities [33]. For this reason, several works are focused in the derivation of stable and high-order schemes [9,10,36]. In [19], Li and Zeng presented a review about GrFD schemes where they discussed their application to different types of fractional differential equations.

Due to the extensive applications of the fractional models, it is necessary to dispose of stable numerical methodologies with high approximation order. In this sense, recent studies have demonstrated that numerical schemes based on Green's functions are alternatives for solving reaction–diffusion equations [35]. In fact, systematic derivation of nonstandard FD schemes can be obtained by means of Green's function formulations [1,15]. In this work a new systematic approach for the discretization of fractional reaction–diffusion equations based on Green's function formulations of the fractional operator is proposed. The numerical solution of proposed scheme is based on method of lines (MOL), where a Runge–Kutta method is used for solving the ordinary differential equations (ODE) system obtained. The paper is organized as follows. First we present the integral formulation of the fractional differential equation [2,32]. Subsequently, a quadrature rule is used to obtain a set of ordinary differential equations. In addition, depending on the discretization of the integral, a numerical scheme with equivalent structure to finite differences based on Grünwald formula can be obtained. To illustrate the numerical accuracy of the method, the results are compared with the analytical and numerical solutions via GrFD.

2. Preliminaries

For convenience, we start our derivations by presenting some definitions and properties of the fractional integral and differential operators [2,32]. Later, we describe the derivation of integral formulation for solving fractional reaction–diffusion systems.

For the study of fractional differential equations, different definitions of the derivatives and integrals have been proposed [29,28,26]. The fractional integral operator of order $\alpha > 0$ of a function $u(x)$ is defined as [2],

$$I_a^{\alpha} u(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x - z)^{\alpha - 1} u(x) dz \tag{1}$$

where I_a^{α} is the so-called Riemann–Liouville fractional integral operator of order α. On the other hand, the fractional differential operator for a function $u(x)$ is defined as [32],

$$D_a^{\alpha} u(x) = \frac{1}{\Gamma(n - \alpha)} \int_a^x (x - z)^{n - \alpha - 1} \frac{d^n u(z)}{dz^n} dz \tag{2}$$

where D_a^{α} is the Caputo derivative of order α and n is an integer such that $n - 1 < \alpha \leq n$. Note that when $\alpha = 2$ one recovers the classical diffusion operator. It is assumed that $u(x)$ is a continuously differentiable function and piecewise smooth, in order for the following considerations to be true [2,32],

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