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Mathematical analysis and numerical simulation of patterns in fractional and classical reaction-diffusion systems

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ABSTRACT

The aim of this paper is to examine pattern formation in the sub– and super-diffusive scenarios and compare it with that of classical or standard diffusive processes in two-component fractional reaction-diffusion systems that modeled a predator-prey dynamics. The focus of the work concentrates on the use of two separate mathematical techniques, we formulate a Fourier spectral discretization method as an efficient alternative technique to solve fractional reaction-diffusion problems in higher-dimensional space, and later advance the resulting systems of ODEs in time with the adaptive exponential time-differencing solver. Obviously, the fractional Fourier approach is able to achieve spectral convergence up to machine precision regardless of the fractional order α, owing to the fact that our approach is able to give full diagonal representation of the fractional operator. The complexity of the dynamics in this system is theoretically discussed and graphically displayed with some examples and numerical simulations in one, two and three dimensions.

1. Introduction

The physical world is apparently described by nonlinear models which either exist in the form of ordinary or partial differential equations. Nonlinear partial differentialequations (PDEs) and most dynamical models display a number of phenomena that are not readily available in the theories of linear systems; a large number of these nonlinear phenomena are apparently related to some important features of the real world situations that are described by the mathematical models in biology and ecology. The study of nonlinear properties especially in the various fields of science and engineering has been and will continue to be a means of arriving at new problems, and that has actually motivated researchers of various disciplines over the years to seek for appropriate methods of solution and analysis of such models.

In this paper, emphasis is given to the numerical solution two components reaction-diffusion (RD) systems: The first is the classical or standard RD system, written in its general form

$$\left.\begin{aligned} \frac{\partial u}{\partial t} &= \delta_1 \Delta u + f(u,v), && \wp \in \Omega, \quad t > 0 \\ \frac{\partial v}{\partial t} &= \delta_2 \Delta u + g(u,v), && \wp \in \Omega, \quad t > 0 \\ \frac{\partial u}{\partial \nu} &= \frac{\partial u}{\partial \nu} = 0, && \wp \in \partial\Omega, \quad t > 0, \\ u(\wp, 0) &= u_0(\wp) \geq 0, && v(\wp, 0) = v_0(\wp) \geq 0, \quad \wp \in \Omega. \end{aligned}\right\} \tag{1.1}$$

where $u(\wp, t)$ and $v(\wp, t)$ are the respective population densities of prey and predators in position (vector) $\wp$ and time t, $\Delta = \frac{\partial^2}{\partial \wp^2}$; $u(\wp, t), v(\wp, t) \in \mathbb{R}$ denotes the two variables Laplacian operator in some space dimensions, whilst δ_1 and δ_2 are strictly positive parameters that represent the diffusion coefficients of both prey and predator. The functions $f(u, v), g(u, v)$ are the nonlinear sources of the system that model their production rates. We assume the domain Ω is bounded and open subset of $\mathbb{R}^d$, $d \leq 3$. The choice of Neumann boundary condition here indicates that the species environment Ω is confined and ν is the outward unit normal to $\partial\Omega$. The initial values $u_0(\wp)$, $v_0(\wp)$ are assumed to be strictly positive and bounded in Ω.

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If E is a subset of $\mathbb{R}^d$ and $\mathbf{f}: E \to \mathbb{R}^n$, $\mathbf{f} := (u, v)$, a function defined on E with values in $\mathbb{R}^n$. Then we propose the following useful definitions:

Definition 1.1. *The function $\mathbf{f}: E \to \mathbb{R}^n$ is continuous at $\mathbf{a} \in E$ if for every neighborhood $V(\mathbf{f}(\mathbf{a}))$ of the value $\mathbf{f}(\mathbf{a})$ that the function assumes at $\mathbf{a}$, $\exists$ a neighborhood $U_E(\mathbf{a})$ of $\mathbf{a}$ in E whose image $\mathbf{f}(U_E(\mathbf{a}))$ is contained in $V(\mathbf{f}(\mathbf{a}))$.*

Thus,

$$(\mathbf{f}: E \to \mathbb{R}^n \text{ is continuous at } \mathbf{a} \in E) := (\forall V(\mathbf{f}(\mathbf{a}))\ \exists U_E(\mathbf{a}) \mathbf{f}(U_E(\mathbf{a})) \subset V(\mathbf{f}(\mathbf{a}))).$$

Definition 1.2. *A domain in $\mathbb{R}^d$ is an open connected set.*

The second model is the fractional-in-space reaction-diffusion system. A space fractional diffusion system can be derived by replacing the second-order spatial derivatives in (1.1) by its fractional counterpart, regarded as the Riemann–Liouville fractional derivatives in space with order α [13,37]

$$\left.\begin{aligned} \frac{\partial u}{\partial t} &= \delta_1 \Delta^{\alpha/2} u + f(u, v), \\ \frac{\partial v}{\partial t} &= \delta_2 \Delta^{\alpha/2} v + g(u, v), \end{aligned}\right\} \tag{1.2}$$

subject to the initial and boundary conditions in (1.1), where δ_1, δ_2 are regarded as the conductivities or diffusion tensors, and $\Delta^\alpha = (\frac{\partial^\alpha}{\partial x^\alpha}, \frac{\partial^\alpha}{\partial y^\alpha}, \frac{\partial^\alpha}{\partial z^\alpha})^{\mathbf{T}}$, $1 < \alpha \le 2$ is the Riemann–Louiville fractional gradient, for

$$\frac{\partial^\alpha}{\partial x^\alpha} u(x, y, z) = \frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial x} \int_0^x \frac{u(s, y, z)}{(x-s)^\alpha} ds,$$

with $\frac{\partial^\alpha}{\partial y^\alpha}$ and $\frac{\partial^\alpha}{\partial z^\alpha}$ having similar expressions.

One of the major advantages of using the Riemann–Liouville fractional derivative within the variation principles is due to the possibility of defining the integration by parts as the fractional reaction-diffusion problems becomes the classical or standard type when α is an integer [2,30]. More importantly, it satisfies all the mathematical principle under the scope of fractional calculus, more importantly when using Laplace transform we obtain initial condition with fractional exponent which is actually realistic in practical and mathematical point of view because we are in the scope of fractional calculus. As a result, most researchers [1,32] endorsed the use of the Riemann–Liouville definition due to its flexibility and suitability.

The study of fractional calculus has a long standing history, from its birth - which has raised a simple question from L'Hospital to Leibnitz - to its today's wide use in many applied scientific fields, fractional calculus has come a long way. In-fact, the field of fractional calculus could be described as old as classical calculus itself. In the last decades, the usefulness of this mathematical theory in applications has gained a lot of weight and has since become more evident and well-pronounced in both field of pure and applied mathematics. In recent times, a lot textbooks and research papers have been published in this active field of research that deal with various aspects in different ways, see for example [15,25–27,34–37]. Also in the past, several numerical techniques have been adopted for solution of fractional reaction-diffusion equations, among them are the work of Fu et al. [7] where a domain-type meshless method in conjunction with finite difference method for constant— and variable-order fractional reaction-diffusion models was used. Based on the Kansa method, the authors in [23] present a domain-type meshless method to solve time fractional reaction-diffusion models. A boundary-only collocation method in conjunction with Laplace transformation to solve time fractional reaction-diffusion models was introduced in [6]. Other numerical techniques designed to solve both time and space fractional reaction-diffusion problems are well classified in [3,5,24] and references therein.

The idea of integral and non-integer differential operators studied in the field of fractional calculus is given by Cauchy's convolution integral

$$\begin{aligned} J^n y(x) &= \int_0^x \int_0^{x_{n-1}} \cdots \int_0^{x_1} y(x_0) dx_0 \cdots dx_{n-2} dx_{n-1} \\ &= \frac{1}{(n-1)!} \int_0^x \frac{1}{(x-t)^{1-n}} y(t) dt, \quad n \in \mathbb{N}, \quad x \in \mathbb{R}_+, \end{aligned}$$

where representation J^n denotes the $n-$fold integer with $J^0 y(x) = y(x)$. When the discrete factorial $(n-1)!$ is replaced with the Euler's gamma function $\Gamma(n)$, for $n \in \mathbb{N}$, we get a definition for a non-integer order integral, that is

$$J^\alpha y(x) = \frac{1}{\Gamma(\alpha)} \int_0^x \frac{1}{(x-t)^{1-\alpha}} y(t) dt, \quad \alpha, x \in \mathbb{R}_+. \tag{1.3}$$

From non-integer derivative (1.3), other important aspects of fractional calculus originate from it, see for example the integer order differentiation and fractional integration

$$D^\alpha y(x) = D^n J^{n-\alpha} y(x) \ \text{ or } \ D_*^\alpha y(x) = J^{n-\alpha} D^n y(x),$$

where n is the integer that satisfies $\alpha \le n < \alpha + 1$ and $D^n, n \in \mathbb{N}$ stands for the $n-$fold differential operator with $D^0 y(x)$. The operator D^α is usually referred to as the Riemann–Liouville operator, while D_*^α is known to be the Caputo differential operator. For preliminary theories and definitions on fractional derivatives, readers are referred to some classical books [15,17,25–27,37].

The interest of this work is devoted to the study of fractional RD (1.2), we only need to compare the results obtained for classical reaction-diffusion equation when $\alpha = 2$ with that of fractional reaction-diffusion system in the range $1 < \alpha \le 2$ called super-diffusion scenario.

The aim of the this paper is to present a Fourier spectral method as an alternative approach to existing finite difference scheme for the numerical solution of (1.2) in one, two and three space dimensions. We also intend to make comparison between the two numerical methods, verify if pattern formation in the diffusive and super-diffusive scenarios are practically the same.

2. Numerical techniques for fractional reaction-diffusion

Spectral methods are applicable whenever high accuracy is required to compute smooth solutions of the partial differential equations. They are valuable for formulating numerical methods in almost all application areas of mathematics, be it in engineering, science and technology. It has ability to spectrally differentiate the fractional derivative operator accurately. Spectral methods are approximation techniques used for the computation of the solutions to both ODEs and PDEs, based on the polynomial expansion of the solution. The precision of these methods is limited only by the regularity of the solution, in contrast to the finite difference method and the finite element methods. The approximation is based primarily on the variational formulation of the continuous problem. The test functions are polynomials and the integrals involved in the formulation are computed by suitable quadrature formulas. This paper proposes to implement a spectral method to solve fractional RD problem.

2.1. Discretization in space

Assume the fractional Laplacian operator $\Delta^{\alpha/2}$ is a complete set of orthonormal eigenfunctions $\{\psi_j\}$ which satisfy the standard boundary conditions defined on a bounded region $\mathcal{D} \subset \mathbb{R}^d, d \le 3$,