UNIVERSIDAD AUTONOMA DE AGUASCALIENTES

CENTRO DE CIENCIAS BÁSICAS

DEPARTAMENTO DE MATEMÁTICAS Y FÍSICA

TESIS

STRUCTURE-PRESERVING METHODS FOR NONLINEAR POPULATION SYSTEMS WITH FRACTIONAL DIFFUSION

PRESENTA

Joel Alba Pérez

PARA OPTAR POR EL GRADO DE DOCTOR EN CIENCIAS APLICADAS Y TECNOLOGÍAS

TUTOR

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Aguascalientes, Ags., October 31, 2023

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PROGRAMA: Doctorado en Ciencias Aplicadas y Tecnología **LGAC (del posgrado):** Matemáticas Aplicadas

TIPO DE TRABAJO: (X) Tesis ( ) Trabajo Práctico

TITULO: STRUCTURE-PRESERVING METHODS FOR NONLINEAR POPULATION SYSTEMS WITH FRACTIONAL DIFFUSION

IMPACTO SOCIAL (señalar el impacto logrado): La tesis presenta diferentes sistemas de ecuaciones diferenciales parciales en multiples dimensiones. Propone métodos basados en diferencias finitas para aproximar las soluciones de estos sistemas de ecuaciones. Los resultados obtenidos son la base de diversos temas en ciencia aplicada.

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Article

Analysis of Structure-Preserving Discrete Models for Predator-Prey Systems with Anomalous Diffusion

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Abstract: In this work, we investigate numerically a system of partial differential equations that describes the interactions between populations of predators and preys. The system considers the effects of anomalous diffusion and generalized Michaelis–Menten-type reactions. For the sake of generality, we consider an extended form of that system in various spatial dimensions and propose two finite-difference methods to approximate its solutions. Both methodologies are presented in alternative forms to facilitate their analyses and computer implementations. We show that both schemes are structure-preserving techniques, in the sense that they can keep the positive and bounded character of the computational approximations. This is in agreement with the relevant solutions of the original population model. Moreover, we prove rigorously that the schemes are consistent discretizations of the generalized continuous model and that they are stable and convergent. The methodologies were implemented efficiently using MATLAB. Some computer simulations are provided for illustration purposes. In particular, we use our schemes in the investigation of complex patterns in some two- and three-dimensional predator–prey systems with anomalous diffusion.

Keywords: systems of parabolic partial differential equations; Riesz space-fractional diffusion; nonlinear population models; structure-preserving methods; stability and convergence analyses

MSC: 65M06; 35K15; 35K55; 35K57

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1. Introduction

The investigation of the interactions between populations of predators and preys in nature is a highly transited topic of research in applied mathematics currently. Indeed, this area of research has proven to be extremely fruitful in view of the wide range of possible scenarios that merit investigation. As examples, we can mention studies that report on the modeling and analysis of predator–prey models with disease in the prey [1], the analysis of stochastic systems with modified Leslie–Gower and Holling-type schemes [2], the dynamic behaviors of Lotka–Volterra predator–prey models that incorporate predator cannibalism [3], the analysis of diffusive predator–prey systems with Michaelis–Menten-type predator harvesting [4], synthetic *Escherichia coli* predator–prey ecosystems [5], the analytical investigation of stage-structured predator–prey models depending on maturation delay and death rate [6], and non-autonomous ratio dependent models with Holling-type functional response with temporal delay [7], among other interesting topics [8].

It is worth pointing out that the investigation has focused mainly on the analytical aspects of the problem [9]. However, the literature reports on various numerical methods that have been designed explicitly to solve efficiently various predator–prey systems. For instance, there are studies

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A positive and bounded convergent scheme for general space-fractional diffusion-reaction systems with inertial times

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ABSTRACT

We consider a multidimensional system of hyperbolic equations with fractional diffusion, constant damping and nonlinear reactions. The system considers fractional Riesz derivatives, and generalizes many models from science. In particular, the system describes the dynamics of populations with temporal delays, whence the need to approximate nonnegative and bounded solutions is an important numerical task. Motivated by these facts, we propose a scheme to approximate the solutions. We prove the existence of the solutions under suitable regularity assumptions on the reaction functions. We prove that the scheme is capable of preserving positivity and boundedness. The technique has consistency of the second order in space and time. Using a discrete form of the energy method, we establish the stability and the convergence. As a corollary, we prove the uniqueness of the solutions. Some computer simulations in the two- and the three-dimensional scenarios are provided at the end of this work for illustration purposes.

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1. Introduction

The design of structure-preserving techniques to solve systems of partial differential equations is an important avenue of research in numerical analysis. In a broadest sense, *structure-preserving techniques* are numerical methods which are able to preserve distinctive features of some relevant solutions of a system of partial differential equations. For example, the relevant solutions of problems involving the growth of populations of bacteria must be nonnegative at all spatial points and at each time [4]. In those cases, solutions which may take on negative values are meaningless, and the condition of positivity is an important feature of the physically realistic solutions of those problems [76]. In other problems, the condition of the boundedness of the solutions may be an important characteristic of the solutions. Such is the case in those problems in which there exist natural limitations for a physical quantity of the problem. In particular, the preservation of the boundedness in systems of partial differential equations describing the growth of colonies of bacteria in a biological culture is a fundamental characteristic of the solutions of those models [44]. Other important features of the solutions of systems of partial differential equations may include the monotonicity [3] and the convexity of solutions [71]. However, the adjective 'structure-preserving' may be applied to any scheme which is capable of preserving an essential feature of the solutions of interest. Nowadays, this concept has been adopted by areas outside of numerical analysis of partial differential equations [1,70,74].

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A finite-difference discretization preserving the structure of solutions of a diffusive model of type-1 human immunodeficiency virus

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Abstract
We investigate a model of spatio-temporal spreading of human immunodeficiency virus HIV-1. The mathematical model considers the presence of various components in a human tissue, including the uninfected CD4$^+$T cells density, the density of infected CD4$^+$T cells, and the density of free HIV infection particles in the blood. These three components are nonnegative and bounded variables. By expressing the original model in an equivalent exponential form, we propose a positive and bounded discrete model to estimate the solutions of the continuous system. We establish conditions under which the nonnegative and bounded features of the initial-boundary data are preserved under the scheme. Moreover, we show rigorously that the method is a consistent scheme for the differential model under study, with first and second orders of consistency in time and space, respectively. The scheme is an unconditionally stable and convergent technique which has first and second orders of convergence in time and space, respectively. An application to the spatio-temporal dynamics of HIV-1 is presented in this manuscript. For the sake of reproducibility, we provide a computer implementation of our method at the end of this work.

MSC: Primary 65M06; secondary 65M22; 65Q10

Keywords: Human immunodeficiency virus; Diffusive mathematical model; Structure-preserving finite-difference scheme

1 Introduction

In this manuscript, we agree that a, b, and T^* are real numbers such that $a < b$ and $T^* > 0$. We fix the spatial domain $B = (a, b)$ and the space-time domain $\Omega = B \times (0, T^*)$. The notation $\overline{\Omega}$ is used to denote the closure of the set Ω in the usual topology of $\mathbb{R}^2$, and we use ∂B to represent the boundary of the set B. In this work, we assume that the functions $T, U, V : \overline{\Omega} \to \mathbb{R}$ are sufficiently smooth. Meanwhile, the constants β, d, k, δ, γ, c, and N represent nonnegative numbers. Also, we define the functions $\phi_T, \phi_U, \phi_V : \overline{B} \to \mathbb{R}$ and $\psi_T, \psi_U, \psi_V : \partial B \times [0, T] \to \mathbb{R}$. Assume additionally that $\phi_W(x) = \psi_W(x, 0)$ holds for each $x \in \partial B$ and $W \in \{T, U, V\}$.

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Joel Alba Pérez

Contents

Resumen

En este manuscrito trabajamos con diferentes sistemas de ecuaciones diferenciales parciales en multiples dimensiones. En estas ecuaciones tomamos el término de difusión y advección como fraccionario de tipo Riesz, y el término de reacción como no lineal. Consideramos condiciones iniciales y de frontera. Existen soluciones analíticas de estas ecuaciones que son complicadas de obtener. Proponemos métodos basados en diferencias finitas para aproximar las soluciones de estos sistemas de ecuaciones. En el primer sistema de ecuaciones consideramos tanto un método implícito como explicito, donde la derivada fraccionaria se encuentra en el término de difusión. El segundo método es un método implicito, donde la derivada fraccionaria está en el término de difusión. El tercer método es un método explicito basado en la técnica de Bhattacharya, en este método no aplicamos derivada fraccionaria. Todos los métodos se basan en el uso de las diferencias centradas fraccionarias, ya que éstas permiten aproximar la derivada fraccionaria de Riesz. Para cada método se estudian sus propiedades estructurales (existencia, unicidad, positividad y acotación) como sus propiedades numéricas (consistencia, estabilidad y convergencia). Por último, para cada método se hacen simulaciones, con el objetivo de ilustrar las aproximaciones a las soluciones analíticas y, además, mostrar que los métodos son capaces de preservar sus propiedades estructurales y numéricas.

Abstract

In this manuscript we work with differents partial differential equations systems in multiple dimensions. In these equations, the diffusion and advection terms are fractional of Riesz type, and the reaction term is nonlinear. We consider the initial–boundary conditions as positive and bounded. The analytical solutions of these equations are difficult to obtain. We propose methods based on finite differences to approximate the solutions of these systems of equations. In the first system of equations we consider an explicit method as an implicit method where the Riesz derivative is in the diffusion term. In the second system of equations we consider an implicit method where the Riesz derivative is in the diffusion term. In the third system of equations we consider an explicit method which is based on the Bhattacharya approach and we will not apply the Riesz derivative. All the methods are based on the use of fractional centered differences, which help us to approximate the Riesz fractional derivatives. For each method, we study the structural properties (existence, uniqueness, positivity and boundedness) and the numerical properties (consistency, stability, and convergence). Finally, for each method, we perform some simulations to depict the numerical approximations. Moreover, we show that all methods are capable to preserve the structural properties.

Introduction

Aims and scope

Differential equations are mathematical tools that help us to study and understand physical, chemical, social, financial and other phenomena that exist in the world. We are interested to work with partial differential equations, even more with systems of partial differential equations, since they help us to study phenomena that are influenced by two or more populations. There are variations to the equations with respect to the order of the derivative, in this thesis we will work with the well known Riesz fractional derivative. This type of derivative allows us to work with non-integer orders, in which we can obtain a better understanding of the phenomenon to be studied. Adding this type of derivative to the system of partial differential equations makes the analytical solution very difficult to obtain, for this reason numerical methods will be applied to approximate the analytical solutions using numerical solutions. We are interested in that the numerical methods that we implement fulfill three important characteristics, the first one is consistency in the analytical model as in the numerical model, the second one is that the solutions are stable and finally, the third one is that the numerical solutions converges to the analytical solutions.

The purpose of this thesis is to work with different systems of partial differential equations where the order of the derivative is fractional. For each system, we will employ an appropriate numerical method to approximate the analytical solutions, thus proving consistency, stability and convergence.

Work Organization

This thesis is sectioned as follows.

- Chapter 1 The investigation of the interactions between populations of predators and preys in nature is a highly transited topic of research in applied mathematics nowadays. Indeed, this area of research has proved to be extremely fruitful in view of the wide range of possible scenarios that merit investigation. As examples, we can mention studies that report on the modeling and analysis of predator-prey models with disease in the prey [1], the analysis of stochastic systems with modified Leslie–Gower and Holling-type schemes [2], the dynamic behaviors of Lotka–Volterra predator-prey models which incorporate predator cannibalism [3], the analysis of diffusive predator-prey systems with Michaelis–Menten-type predator harvesting [4], synthetic Escherichia coli predator-prey ecosystems [5], the analytical investigation of stage structured predator-prey models depending on maturation delay and death rate [6] and non-autonomous ratio-dependent models with Holling-type functional response with temporal delay [7], among other interesting topics.

The system consists of two partial differential equations with coupled reaction terms and Riesz fractional diffusion. We introduce therein the notion of fractional centered differences, which will be the cornerstone to provide a discretization of our model. In turn, we present the discrete nomenclature along with two finite-difference schemes to approximate the solutions of the continuous system. It is worth noting that one of the models will be an implicit scheme, while the second is explicit. These numerical methods will be analyzed structurally. As the most important results from that section, we establish the existence, uniqueness, positivity and boundedness of the solutions for both methods. We devoted to establishing the numerical properties of the schemes, including the consistency, stability and convergence. Some numerical simulations are provided and we close this work with some concluding remarks.

- Chapter 2 we will investigate a general mathematical model consisting of hyperbolic partial differential equations that include the presence of nonlinear reaction terms. The system is sufficiently broad to describe many mathematical models in biology, physics and chemistry. In particular, the model may be employed to describe the space-time interactions of different populations, like diffusive predator-prey systems with an Allee effect in the prey and temporal delays [8]. As a consequence, it is indispensable to be able to guarantee the preservation of the positivity of the solutions. Motivated by these facts, we will propose a positivity- and boundedness-preserving finite-difference scheme to approximate the solutions of our system. The numerical model will be a nonlinear technique, and we will establish the existence of solutions using Brouwer's fixed-point theorem. Moreover, the capability of our scheme to preserve the positive and bounded character of the solutions will be established rigorously after imposing adequate conditions on the discretized reaction terms. In summary, a structure-preserving method (more concretely, a positivity- and boundedness-preserving discrete model) will be proposed to solve our continuous problem.

  To make our approach even more general, the mathematical system considered in this work will include fractional diffusion of the Riesz type [9, 10, 11, 12]. In recent years, fractional differential equations have been used in physical models to obtain more precise descriptions of real-life phenomena [13, 14, 15, 16]. As a consequence, various authors have applied fractional calculus to problems in a wide range of scientific areas [17, 18], including some phenomena of viscoelasticity [19], problems associated to thermoelasticity [20], the modeling in mathematical finance [21], dynamical systems consisting of self-similar proteins [22], quantum field theory [23], the control of diabetes [24], the theory of solitary waves [25] and the physics of plasma [26]. Moreover, the investigation of population systems [27] and, in particular, the modeling of the interactions between populations of predators and preys, has also seen a substantial progress derived from the use of fractional calculus. Indeed, some recent works have investigated fractional predator-prey systems which incorporate feedback control and a constant prey refuge [28], bifurcations of delayed fractional systems with incommensurate orders [29], periodic solutions and control optimization of models with two types of harvesting [30], fractional predator-prey systems with delay and Holling type-II functional response [31], among other recent works available in the literature. It is well known that fractional systems are computationally mode difficult to solve than classical integer-order models. In that sense, the search for computationally efficient algorithms to simulate fractional systems is still open problem of investigation. It is worth pointing out that the conciliation of numerical and computational efficiency is a hard problem to be solved in a completely satisfactory manner. In the present work, we will focus on p-dimensional Euclidean space.

- Chapter 3 We investigate a model of spatio-temporal spreading of human immunodeficiency virus HIV-1. The mathematical model considers the presence of various components in a human tissue, including the unifected CD4 T cells density, the density of infected CD4 T cells, and the density of free HIV infection particles in the blood. These three components are nonnegtive and bounded variables. By expressing the original model in an equivalent exponential form, we propose a positive and bounded discrete model to estimate the solutions of the continuous system. We establish conditions under which the nonnegative and bounded features of the initial-boundary data are preserved under the scheme for the differential model under study, with first and second orders of consistency in time and space, respectively. The scheme is an unconditionally stable and convergent technique which has first and second orders of convergence in time and space, respectively.

1. Analysis of Structure-Preserving Discrete Models for Predator-Prey Systems with Anomalous Diffusion

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Analysis of Structure-Preserving Discrete Models for Predator-Prey Systems with Anomalous Diffusion

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Abstract: In this work, we investigate numerically a system of partial differential equations that describes the interactions between populations of predators and preys. The system considers the effects of anomalous diffusion and generalized Michaelis–Menten-type reactions. For the sake of generality, we consider an extended form of that system in various spatial dimensions and propose two finite-difference methods to approximate its solutions. Both methodologies are presented in alternative forms to facilitate their analyses and computer implementations. We show that both schemes are structure-preserving techniques, in the sense that they can keep the positive and bounded character of the computational approximations. This is in agreement with the relevant solutions of the original population model. Moreover, we prove rigorously that the schemes are consistent discretizations of the generalized continuous model and that they are stable and convergent. The methodologies were implemented efficiently using MATLAB. Some computer simulations are provided for illustration purposes. In particular, we use our schemes in the investigation of complex patterns in some two- and three-dimensional predator–prey systems with anomalous diffusion.

Keywords: systems of parabolic partial differential equations; Riesz space-fractional diffusion; nonlinear population models; structure-preserving methods; stability and convergence analyses

MSC: 65M06; 35K15; 35K55; 35K57

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1. Introduction

The investigation of the interactions between populations of predators and preys in nature is a highly transited topic of research in applied mathematics currently. Indeed, this area of research has proven to be extremely fruitful in view of the wide range of possible scenarios that merit investigation. As examples, we can mention studies that report on the modeling and analysis of predator–prey models with disease in the prey [1], the analysis of stochastic systems with modified Leslie–Gower and Holling-type schemes [2], the dynamic behaviors of Lotka–Volterra predator–prey models that incorporate predator cannibalism [3], the analysis of diffusive predator–prey systems with Michaelis–Menten-type predator harvesting [4], synthetic *Escherichia coli* predator–prey ecosystems [5], the analytical investigation of stage-structured predator–prey models depending on maturation delay and death rate [6], and non-autonomous ratio dependent models with Holling-type functional response with temporal delay [7], among other interesting topics [8].

It is worth pointing out that the investigation has focused mainly on the analytical aspects of the problem [9]. However, the literature reports on various numerical methods that have been designed explicitly to solve efficiently various predator–prey systems. For instance, there are studies on dynamically consistent nonstandard finite-difference schemes to solve predator–prey models [10], while some of those methods have been implemented in MATLAB with the aim of being available to the scientific community [11]. There are also some positive and elementary stable nonstandard schemes that have been applied to solve predator–prey systems [12], modified Leslie–Gower and Holling-type II schemes with temporal delay [13], nonstandard numerical schemes for predator–prey models having a generalized functional response [14], as well as positivity and boundedness-preserving methods for some space-time fractional predator–prey models [15]. Of course, the investigation in this area is still an important topic of research.

To date, fractional differential equations have been used in mathematical systems to produce more accurate models for physical problems [16]. Various applications have been proposed in a number of areas [17,18], including various problems in viscoelasticity [19], some phenomena related to thermoelasticity [20], in continuous-time financing problems [21], in the dynamics of self-similar proteins [22], relativistic quantum mechanics [23], the control of diabetes [24], the theory of solitons [25], and plasma physics [26]. Moreover, the research on predator–prey systems has also benefited from the recent progresses in fractional calculus. Recent reports have studied fractional models of predators and preys that incorporate feedback control and a constant prey refuge [27], bifurcations of delayed fractional systems with incommensurate orders [28], periodic solutions and control optimization of models with two types of harvesting [29], and fractional predator–prey systems with delay and Holling type-II functional response [30], among other recent works available in the literature.

It is well known that the complexity of fractional systems is much higher than the complexity of integer-order systems. From that point of view, it is necessary to propose efficient numerical methods to solve meaningful fractional-order systems [31]. In that sense, the literature provides some reports to calculate the solutions of fractional models. For instance, there are some computational schemes to approximate the solutions of fractional differential equations using fractional centered differences [32], the diffusion equation with fractional derivatives in time [33], the multidimensional fractional Schrödinger equation [34], the nonlinear Korteweg–de Vries–Burgers equation with fractional derivatives [35], and the two-dimensional fractional FitzHugh–Nagumo monodomain model [36], among others [37]. However, the search for better algorithms to simulate fractional systems (which provide fast results with minimal computer resources) is still an open problem of research.

Motivated by this background, we will consider a predator–prey system with fractional diffusion that considers reaction functionals. The reaction terms will follow Michaelis–Menten laws [38], while the diffusion considered in this work will be of the Riesz type [39]. It is worth pointing out here that the choice of the fractional derivative type obeys various mathematical and physical reasons. Most importantly, it has been recently found that Riesz fractional derivatives can be obtained from systems with long range interactions in some continuous-limit approximations [40]. In order to reach some level of generality, we will consider an extended form of the predator–prey system under investigation, considering sufficiently general reaction functions and various spatial dimensions. In light of the complexity to solve exactly such a model, we will propose some finite-difference methods based on the concept of fractional centered differences [41]. Motivated then by the fact that the relevant solutions of the system are positive and bounded functions, we will prove that our discretizations are capable of preserving these features of the numerical solutions. Moreover, we will prove rigorously the consistency, the stability, and the convergence of the methodologies. Some applications will be provided to illustrate the usefulness of our models and our implementations.

This manuscript is sectioned as follows. In Section 2, we provide the mathematical system under study. The system consists of two partial differential equations with coupled reaction terms and Riesz fractional diffusion. We introduce therein the definition of fractional centered differences, which is the cornerstone to provide a discretization of our model. In turn, Section 3 presents the discrete notation along with two finite-difference schemes to estimate the solutions of the continuous system. It is worth noting that one of the models will be an implicit scheme, while the other is explicit. These numerical methods will be analyzed structurally in Section 4. As the most important results from that section, we establish the existence, uniqueness, positivity, and boundedness of the solutions for both methods. Section 5 is devoted to establishing the numerical properties of the schemes, including the consistency, stability, and convergence. Some numerical applications are provided in Section 6, and we close this manuscript with some concluding observations.

2. Preliminaries

Throughout, assume that a_i and b_i are real numbers such that $a_i < b_i$, for each $i = 1, 2, 3$. Let $T > 0$ represent a fixed time. We define $\Omega = (a_1, b_1) \times (a_2, b_2) \times (a_3, b_3)$ and $\Omega_T = \Omega \times (0, T)$ and use $\overline{\Omega}$ and $\overline{\Omega}_T$ to represent the closures of Ω and Ω_T, respectively. In this manuscript, $u : \overline{\Omega}_T \to \mathbb{R}$ and $v : \overline{\Omega}_T \to \mathbb{R}$ represent sufficiently smooth functions, and define $x = (x_1, x_2, x_3) \in \Omega$.

Definition 1 (Podlubny [42])**.** *Assume that $f : \mathbb{R} \to \mathbb{R}$, and suppose that $n \in \mathbb{N} \cup \{0\}$ and $\alpha \in \mathbb{R}$ are such that $n - 1 < \alpha < n$. If it exists, we introduce the fractional derivative in the sense of Riesz of the function f of order α at the point $x \in \mathbb{R}$ as:*

$$\frac{d^\alpha f(x)}{d|x|^\alpha} = \frac{-1}{2\cos(\frac{\pi\alpha}{2})\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_{-\infty}^{\infty} \frac{f(\xi)d\xi}{|x-\xi|^{\alpha+1-n}}. \tag{1}$$

Here, the Gamma function is given by:

$$\Gamma(z) = \int_0^\infty s^{z-1} e^{-s} ds, \qquad \forall z > 0. \tag{2}$$

Definition 2. *Suppose that $u : \overline{\Omega}_T \to \mathbb{R}$; assume that $\alpha > -1$; and let $n \in \mathbb{Z}$ satisfy $n - 1 < \alpha \leq n$. If they exist, the Riesz space-fractional derivatives of the function u of order α with respect to x_1, x_2, and x_3 at the point $(x, t) \in \Omega_T$ are respectively defined by:*

$$\frac{\partial^\alpha u}{\partial|x_1|^\alpha}(x,t) = \frac{-1}{2\cos\left(\frac{\pi\alpha}{2}\right)\Gamma(n-\alpha)} \frac{\partial^n}{\partial x_1^n} \int_{a_1}^{b_1} \frac{u(\xi, x_2, x_3, t)\, d\xi}{|x_1-\xi|^{\alpha+1-n}}, \tag{3}$$

$$\frac{\partial^\alpha u}{\partial|x_2|^\alpha}(x,t) = \frac{-1}{2\cos\left(\frac{\pi\alpha}{2}\right)\Gamma(n-\alpha)} \frac{\partial^n}{\partial x_2^n} \int_{a_2}^{b_2} \frac{u(x_1, \xi, x_3, t)\, d\xi}{|x_2-\xi|^{\alpha+1-n}}, \tag{4}$$

$$\frac{\partial^\alpha u}{\partial|x_3|^\alpha}(x,t) = \frac{-1}{2\cos\left(\frac{\pi\alpha}{2}\right)\Gamma(n-\alpha)} \frac{\partial^n}{\partial x_3^n} \int_{a_3}^{b_3} \frac{u(x_1, x_2, \xi, t)\, d\xi}{|x_3-\xi|^{\alpha+1-n}}. \tag{5}$$

For the remainder of this paper, we will let a, c, d, D_1, and D_2 be positive; suppose that $b \in \mathbb{R}$, and let $\alpha, \beta \in \mathbb{R}$ be such that $1 < \alpha \leq 2$ and $1 < \beta \leq 2$. Let $\phi_u : \overline{\Omega} \to \mathbb{R}$ and $\phi_v : \overline{\Omega} \to \mathbb{R}$ be two functions that physically describe the initial conditions for populations of prey and predator, respectively. Under these conventions, the problem under investigation is the predator–prey model with Allee effects and diffusion of fractional order, which is described by:

$$\begin{aligned}
&\frac{\partial u(x,t)}{\partial t} = au(u-b)(1-u) - \frac{uv}{u+v} + D_1 \sum_{i=1}^{3} \frac{\partial^\alpha u(x,t)}{\partial|x_i|^\alpha}, \qquad \forall (x,t) \in \Omega_T, \\
&\frac{\partial v(x,t)}{\partial t} = \frac{cuv}{u+v} - dv + D_2 \sum_{i=1}^{3} \frac{\partial^\beta u(x,t)}{\partial|x_i|^\beta}, \qquad \forall (x,t) \in \Omega_T, \\
&\text{such that } \begin{cases} u(x,0) = \phi_u(x), & \forall x \in \Omega, \\ v(x,0) = \phi_v(x), & \forall x \in \Omega. \end{cases}
\end{aligned} \tag{6}$$

Convey that $u = u(x,t)$ and $v = v(x,t)$ for simplicity. The model (6) is a Michaelis–Menten-type reaction-diffusion predator–prey system where the diffusion is anomalous. Here, $u(x,t)$ and $v(x,t)$ represent the normalized densities of the prey and the predator, respectively, at the point $x \in \Omega$ and time $t \geq 0$. The relative constant a is the intrinsic rate of growth of the prey; $b \in (-1,1)$ is the Allee effect; $c \in (0,1]$ denotes the rate of the energy rate from the prey to the predator; and d is the relative rate of death of the predator population. Meanwhile, D_1 and D_2 are non-negative constants that represent the speed of individual movements of u and v, respectively [43].

Notice that we can rewrite the system (6) in generalized form as:

$$\begin{aligned}
&\frac{\partial u(x,t)}{\partial t} = auF(u) - uG^u(u,v) + D_1 \sum_{i=1}^{3} \frac{\partial^\alpha u(x,t)}{\partial |x_i|^\alpha}, \qquad \forall (x,t) \in \Omega_T, \\
&\frac{\partial v(x,t)}{\partial t} = cvG^v(u,v) - dv + D_2 \sum_{i=1}^{3} \frac{\partial^\beta v(x,t)}{\partial |x_i|^\beta}, \qquad \forall (x,t) \in \Omega_T, \\
&\text{such that } \begin{cases} u(x,0) = \phi_u(x), & \forall x \in \Omega, \\ v(x,0) = \phi_v(x), & \forall x \in \Omega. \end{cases}
\end{aligned} \tag{7}$$

where the function F depends on u, while G^u and G^v depend on both u and v. It is easy to see that the system (7) reduces to the population model (6) when F, G^u, and G^v have the following expressions with $u, v \in \mathbb{R}^+ \cup \{0\}$:

$$F(u) = (u-b)(1-u), \qquad G^u(u,v) = \frac{v}{u+v}, \qquad G^v(u,v) = \frac{u}{u+v}. \tag{8}$$

Moreover, if $\alpha = \beta = 2$, $D_1 = D_2 = 0$, $F(u,v) = 1$, $G^u = v$, and $G^v = u$, then (7) reduces to the well-known Lotka–Volterra system.

We recall the following definition from the literature. It will be an essential tool to provide consistent discretizations of the general fractional problem (7).

Definition 3 (Ortigueira [41])**.** *Let $f : \mathbb{R} \to \mathbb{R}$, and assume that $h > 0$ and $\alpha > -1$. The centered difference of fractional order α of the function f at x is given (when it exists) as:*

$$\Delta_h^{(\alpha)} f(x) = \sum_{k=-\infty}^{\infty} g_k^{(\alpha)} f(x - kh), \qquad \forall x \in \mathbb{R}, \tag{9}$$

where:

$$g_k^{(\alpha)} = \frac{(-1)^k \Gamma(\alpha+1)}{\Gamma(\frac{\alpha}{2} - k + 1)\Gamma(\frac{\alpha}{2} + k + 1)}, \qquad \forall k \in \mathbb{Z}. \tag{10}$$

Lemma 1 (Wang et al. [44])**.** *Let $0 < \alpha \leq 2$ and $\alpha \neq 1$.*

(a) *The following iterative formulas hold:*

$$g_0^{(\alpha)} = \frac{\Gamma(\alpha+1)}{[\Gamma(\frac{\alpha}{2}+1)]^2}, \tag{11}$$

$$g_{k+1}^{(\alpha)} = \left(1 - \frac{\alpha+1}{\alpha/2 + k + 1}\right) g_k, \qquad \forall k \in \mathbb{N} \cup \{0\}. \tag{12}$$

(b) $g_0^{(\alpha)} > 0$.
(c) $g_k^{(\alpha)} = g_{-k}^{(\alpha)} < 0$ *for all* $k \neq 0$.
(d) $\sum_{k=-\infty}^{\infty} g_k^{(\alpha)} = 0$.

Lemma 2 (Wang et al. [44])**.** *Let $0 < \alpha \leq 2$ and $\alpha \neq 1$, and suppose that $f \in \mathcal{C}^5(\mathbb{R})$ is a function whose derivatives up to order five are all integrable. For almost all $x \in \mathbb{R}$,*

$$-\frac{\Delta_h^\alpha f(x)}{h^\alpha} = \frac{\partial^\alpha f(x)}{\partial |x|^\alpha} + \mathcal{O}(h^2). \tag{13}$$

3. Numerical Models

The purpose of this section is to propose two different methods based on finite-differences to approximate the solutions of (7). For the sake of convenience, we consider only the two-dimensional form of (7), which reads as follows:

$$\begin{aligned}
&\frac{\partial u(x,t)}{\partial t} = auF(u) - uG^u(u,v) + D_1 \sum_{i=1}^{2} \frac{\partial^\alpha u(x,t)}{\partial |x_i|^\alpha}, \qquad \forall (x,t) \in \Omega_T, \\
&\frac{\partial v(x,t)}{\partial t} = cvG^v(u,v) - dv + D_2 \sum_{i=1}^{2} \frac{\partial^\beta v(x,t)}{\partial |x_i|^\beta}, \qquad \forall (x,t) \in \Omega_T, \\
&\text{such that } \begin{cases} u(x,0) = \phi_u(x), & \forall x \in \Omega, \\ v(x,0) = \phi_v(x), & \forall x \in \Omega. \end{cases}
\end{aligned} \tag{14}$$

It is worth pointing out that an analysis of the three-dimensional model is also feasible, though it would require additional nomenclature. We preferred to carry out the full description and analysis in the two-dimensional case for the sake of a better explanation.

Agree that $I_p = \{1, 2, \ldots, p\}$ and $\bar{I}_p = I_p \cup \{0\}$, for all $p \in \mathbb{N}$. Let $M, N, K \in \mathbb{N}$, and introduce uniform partitions of $[a_1, b_1]$ and $[a_2, b_2]$, respectively, denoted by:

$$\begin{aligned}
a_1 = x_{1,0} < x_{1,1} < \ldots < x_{1,m} < \ldots < x_{1,M} = b_1, \quad \forall m \in \bar{I}_M, \\
a_2 = x_{2,0} < x_{2,1} < \ldots < x_{2,n} < \ldots < x_{2,N} = b_2, \quad \forall n \in \bar{I}_N.
\end{aligned} \tag{15}$$

Obviously, $x_{1,m} = a_1 + h_{x_1} m$ and $x_{2,n} = a_2 + h_{x_2} n$ for each $m \in \bar{I}_M$ and $n \in \bar{I}_N$. In this case, the partition norms in the x_1 and x_2 directions are $h_{x_1} = (b_1 - a_1)/M$ and $h_{x_2} = (b_2 - a_2)/N$, respectively.

In a similar fashion, we fix a (not necessarily uniform) partition for the interval $[0, T]$, which will be represented by:

$$0 = t_0 < t_1 < \ldots < t_k < \ldots < t_K = T, \quad \forall k \in \bar{I}_K. \tag{16}$$

For each $k \in \bar{I}_{K-1}$, we let $\tau_k = t_{k+1} - t_k$. Numerically, we define $u^k_{m,n}$ and $v^k_{m,n}$, respectively, as the approximations to the analytical solutions u and v of (14) at the point $(x_{1,m}, x_{2,n}, t_k)$ for each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in \bar{I}_K$.

Definition 4. *Let $\alpha \in (0,1) \cup (1,2]$. Define the discrete linear operators:*

$$\delta^{(\alpha)}_{x_1} u^k_{m,n} = -\frac{1}{h^\alpha_{x_1}} \sum_{i=0}^{M} g^{(\alpha)}_{m-i} u^k_{i,n}, \qquad \delta^{(\alpha)}_{x_2} u^k_{m,n} = -\frac{1}{h^\alpha_{x_2}} \sum_{i=0}^{N} g^{(\alpha)}_{n-i} u^k_{m,i}, \tag{17}$$

$$\delta^{(\alpha)}_{x_1} v^k_{m,n} = -\frac{1}{h^\alpha_{x_1}} \sum_{i=0}^{M} g^{(\alpha)}_{m-i} v^k_{i,n}, \qquad \delta^{(\alpha)}_{x_2} v^k_{m,n} = -\frac{1}{h^\alpha_{x_2}} \sum_{i=0}^{N} g^{(\alpha)}_{n-i} v^k_{m,i}. \tag{18}$$

By Lemma 2, the discrete operators introduced above provide approximations of second order to the Riesz spatial derivatives of the functions u and v, with respect to x_1 and x_2 at the point $(x_{1,m}, x_{2,n}, t_k)$. For the remainder of this work and without loss of generality, we assume that the partition of the interval $[0, T]$ is uniform, in which case $\tau_k = \tau \in \mathbb{R}^+$, for each $k \in \bar{I}_{K-1}$. This assumption will be imposed only for the sake of convenience in the use of our notation.

3.1. Explicit Method

We present here an explicit scheme to approximate the solutions of (14). In the first stage, we introduce additional discrete operators to describe the scheme. The nomenclature presented in Section 2 will be observed throughout this section.

Definition 5. *Let w be any of u or v. For each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$, we introduce the standard linear operators:*

$$\delta_t w_{m,n}^k = \frac{w_{m,n}^{k+1} - w_{m,n}^k}{\tau}, \tag{19}$$

Recall now that the operator (19) yields a first-order estimate of the partial derivative of w with respect to time at $(x_{1,m}, x_{2,n}, t)$, for each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$. Substituting the differential operators of (7) for their finite-difference approximations, we obtain the following discrete model to approximate the solutions of (14):

$$\begin{aligned} \delta_t u_{m,n}^k &= aF(u_{m,n}^k)u_{m,n}^k - G^u(u_{m,n}^k, v_{m,n}^k)u_{m,n}^k + D_1 \sum_{i=1}^{2} \delta_{x_i}^{(\alpha)} u_{m,n}^k, \\ \delta_t v_{m,n}^k &= cG^v(u_{m,n}^k, v_{m,n}^k)v_{m,n}^k - dv_{m,n}^k + D_2 \sum_{i=1}^{2} \delta_{x_i}^{(\beta)} v_{m,n}^k, \\ \text{such that } & \left\{ \begin{array}{ll} u_{m,n}^0 = \phi_{u,m,n}^0, & \forall (m,n) \in \bar{I}_M \times \bar{I}_N, \\ v_{m,n}^0 = \phi_{v,m,n}^0, & \forall (m,n) \in \bar{I}_M \times \bar{I}_N. \end{array} \right. \end{aligned} \tag{20}$$

Here, the difference equations are valid for each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in \bar{I}_{K-1}$.

Substituting then the expressions of the discrete operators into (20), we obtain an alternative representation of our finite-difference scheme. More precisely, let:

$$R_i^u = \frac{\tau D_1}{h_{x_i}^\alpha} \quad \text{and} \quad R_i^v = \frac{\tau D_2}{h_{x_i}^\beta}, \tag{21}$$

for each $i = 1, 2$ and $\alpha, \beta \in (1, 2]$. After some algebraic operations, it is easy to check that the recursive equations of (20) can be rewritten equivalently as:

$$\begin{aligned} u_{m,n}^{k+1} &= \mathfrak{a}_{m,n}^k u_{m,n}^k + \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{b}_{m,i} u_{i,n}^k + \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{c}_{n,i} u_{m,i}^k, \\ v_{m,n}^{k+1} &= \mathfrak{e}_{m,n}^k v_{m,n}^k + \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{f}_{m,i} v_{i,n}^k + \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{g}_{n,i} v_{m,i}^k, \end{aligned} \tag{22}$$

where:

$$\mathfrak{a}_{m,n}^k = 1 + a\tau F(u_{m,n}^k) - \tau G^u(u_{m,n}^k, v_{m,n}^k) - R_1^u g_0^{(\alpha)} - R_2^u g_0^{(\alpha)}, \tag{23}$$

$$\mathfrak{b}_{m,i} = -R_1^u g_{m-i}^{(\alpha)}, \tag{24}$$

$$\mathfrak{c}_{n,i} = -R_2^u g_{n-i}^{(\alpha)}, \tag{25}$$

$$\mathfrak{e}_{m,n}^k = 1 + \tau c G^v(u_{m,n}^k, v_{m,n}^k) - d\tau - R_1^v g_0^{(\beta)} - R_2^v g_0^{(\beta)}, \tag{26}$$

$$\mathfrak{f}_{m,i} = -R_1^v g_{m-i}^{(\beta)}, \tag{27}$$

$$\mathfrak{g}_{n,i} = -R_2^v g_{n-i}^{(\beta)}. \tag{28}$$

Let $^\top$ represent matrix transposition. Observe then that (22) can be represented in an equivalent vector form. Indeed, let $k \in \bar{I}_K$ and $j \in \bar{I}_M$, and define the $(N+1)$-dimensional vectors:

$$u_j^k = (u_{j,0}^k, u_{j,1}^k, \cdots, u_{j,N-1}^k, u_{j,N}^k)^\top, \tag{29}$$

$$v_j^k = (v_{j,0}^k, v_{j,1}^k, \cdots, v_{j,N-1}^k, v_{j,N}^k)^\top, \tag{30}$$

$$\phi^0_{u,j} = (\phi^0_{u,j,0}, \phi^0_{u,j,1}, \cdots, \phi^0_{u,j,N-1}, \phi^0_{u,j,N})^\top, \tag{31}$$
$$\phi^0_{v,j} = (\phi^0_{v,j,0}, \phi^0_{v,j,1}, \cdots, \phi^0_{v,j,N-1}, \phi^0_{v,j,N})^\top. \tag{32}$$

With these conventions, we introduce the $(M+1) \times (N+1)$-dimensional vectors:

$$u^k = u^k_0 \oplus u^k_1 \oplus \cdots \oplus u^k_M, \tag{33}$$
$$v^k = v^k_0 \oplus v^k_1 \oplus \cdots \oplus v^k_M, \tag{34}$$
$$\phi^0_u = \phi^0_{u,0} \oplus \phi^0_{u,1} \oplus \cdots \oplus \phi^0_{u,M}, \tag{35}$$
$$\phi^0_v = \phi^1_{u,0} \oplus \phi^1_{u,1} \oplus \cdots \oplus \phi^1_{u,M}, \tag{36}$$

where $\oplus$ represents the vector operation of juxtaposition.

The following are all matrices of dimension $(N+1) \times (N+1)$, for each $m \in \overline{I}_M$ and $k \in \overline{I}_{K-1}$:

$$B_{m,i} = \begin{pmatrix} \mathfrak{b}_{m,i} & 0 & 0 & \cdots & 0 \\ 0 & \mathfrak{b}_{m,i} & 0 & \cdots & 0 \\ 0 & 0 & \mathfrak{b}_{m,i} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \mathfrak{b}_{m,i} \end{pmatrix}, \quad C^k_m = \begin{pmatrix} \mathfrak{a}^k_{m,0} & \mathfrak{c}_{0,1} & \mathfrak{c}_{0,2} & \cdots & \mathfrak{c}_{0,N} \\ \mathfrak{c}_{1,0} & \mathfrak{a}^k_{m,1} & \mathfrak{c}_{1,2} & \cdots & \mathfrak{c}_{1,N} \\ \mathfrak{c}_{2,0} & \mathfrak{c}_{2,1} & \mathfrak{a}^k_{m,2} & \cdots & \mathfrak{c}_{2,N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathfrak{c}_{N,0} & \mathfrak{c}_{N,1} & \mathfrak{c}_{N,2} & \cdots & \mathfrak{a}^k_{m,N} \end{pmatrix}, \tag{37}$$

$$F_{m,i} = \begin{pmatrix} \mathfrak{f}_{m,i} & 0 & 0 & \cdots & 0 \\ 0 & \mathfrak{f}_{m,i} & 0 & \cdots & 0 \\ 0 & 0 & \mathfrak{f}_{m,i} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \mathfrak{f}_{m,i} \end{pmatrix}, \quad G^k_m = \begin{pmatrix} \mathfrak{e}^k_{m,0} & \mathfrak{g}_{0,1} & \mathfrak{g}_{0,2} & \cdots & \mathfrak{g}_{0,N} \\ \mathfrak{g}_{1,0} & \mathfrak{e}^k_{m,1} & \mathfrak{g}_{1,2} & \cdots & \mathfrak{g}_{1,N} \\ \mathfrak{g}_{2,0} & \mathfrak{g}_{2,1} & \mathfrak{e}^k_{m,2} & \cdots & \mathfrak{g}_{2,N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathfrak{g}_{N,0} & \mathfrak{g}_{N,1} & \mathfrak{g}_{N,2} & \cdots & \mathfrak{e}^k_{m,N} \end{pmatrix}. \tag{38}$$

For each $k \in \overline{I}_{K-1}$, let A^k_u and A^k_v be block matrices of sizes $[(M+1) \times (N+1)] \times [(M+1) \times (N+1)]$, which are defined respectively by:

$$A^k_u = \begin{pmatrix} C^k_0 & B_{0,1} & B_{0,2} & \cdots & B_{0,M} \\ B_{1,0} & C^k_1 & B_{1,2} & \cdots & B_{1,M} \\ B_{2,0} & B_{2,1} & C^k_2 & \cdots & B_{2,M} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_{M,0} & B_{M,1} & B_{M,2} & \cdots & C^k_M \end{pmatrix}, \quad A^k_v = \begin{pmatrix} G^k_0 & F_{0,1} & F_{0,2} & \cdots & F_{0,M} \\ F_{1,0} & G^k_1 & F_{1,2} & \cdots & F_{1,M} \\ F_{2,0} & F_{2,1} & G^k_2 & \cdots & F_{2,M} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ F_{M,0} & F_{M,1} & F_{M,2} & \cdots & G^k_M \end{pmatrix}. \tag{39}$$

With this notation, the vector representation of (22) is given by the iterative system:

$$\begin{aligned} u^{k+1} &= A^k_u u^k, \quad \forall k \in I_{K-1}, \\ v^{k+1} &= A^k_v v^k, \quad \forall k \in I_{K-1}, \\ \text{such that} & \begin{cases} u^0 = \phi^0_u, \\ v^0 = \phi^0_v. \end{cases} \end{aligned} \tag{40}$$

3.2. Implicit Method

The purpose of this section is to introduce a Crank–Nicolson-type technique to approximate the solutions of (14). In the first stage, we define some discrete operators used to design our implicit finite-difference scheme. In the present section, we will observe the notation presented previously. The purpose is to provide various equivalent representations of the Crank–Nicolson scheme, which will be mathematically useful.

Definition 6. *Let w be any of u or v. For each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$, we introduce the discrete linear operators:*

$$\delta_t^{(1)} w_{m,n}^k = \frac{w_{m,n}^{k+1} - w_{m,n}^{k-1}}{2\tau} \qquad \text{and} \qquad \mu_t^{(1)} w_{m,n}^k = \frac{w_{m,n}^{k+1} + w_{m,n}^{k-1}}{2}. \tag{41}$$

Remember that the discrete operators introduced in the previous definition yield second-order estimates of the temporal partial derivative of w at the point $(x_{1,m}, x_{2,n}, t)$ and the exact value of w at that point, respectively. With this notation, a second finite-difference methodology to calculate the solutions of (14) is provided by the implicit system:

$$\begin{aligned}
\delta_t^{(1)} u_{m,n}^k &= aF(u_{m,n}^k)\mu_t^{(1)} u_{m,n}^k - G^u(u_{m,n}^k, v_{m,n}^k)\mu_t^{(1)} u_{m,n}^k + D_1 \sum_{i=1}^{2} \mu_t^{(1)} \delta_{x_i}^{(\alpha)} u_{m,n}^k, \\
\delta_t^{(1)} v_{m,n}^k &= cG^v(u_{m,n}^k, v_{m,n}^k)\mu_t^{(1)} v_{m,n}^k - d\mu_t^{(1)} v_{m,n}^k + D_2 \sum_{i=1}^{2} \mu_t^{(1)} \delta_{x_i}^{(\beta)} v_{m,n}^k, \\
&\text{such that } \begin{cases} u_{m,n}^0 = \phi_{u,m,n}^0, & \forall (m,n) \in \bar{I}_M \times \bar{I}_N, \\ u_{m,n}^1 = \phi_{u,m,n}^1, & \forall (m,n) \in \bar{I}_M \times \bar{I}_N, \\ v_{m,n}^0 = \phi_{v,m,n}^0, & \forall (m,n) \in \bar{I}_M \times \bar{I}_N, \\ v_{m,n}^1 = \phi_{v,m,n}^1, & \forall (m,n) \in \bar{I}_M \times \bar{I}_N, \end{cases}
\end{aligned} \tag{42}$$

for each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$.

As in the case of the explicit method, an equivalent implicit representation of (42) is readily at hand. Indeed, after some algebraic simplifications and convenient manipulations, the difference equations of the system (42) can be rewritten as:

$$\begin{aligned}
\mathfrak{a}_{m,n}^k u_{m,n}^{k+1} + \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{b}_{m,i} u_{i,n}^{k+1} + \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{c}_{n,i} u_{m,i}^{k+1} &= (2 - \mathfrak{a}_{m,n}^k) u_{m,n}^{k-1} + \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{b}_{m,i} u_{i,n}^{k-1} + \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{c}_{n,i} u_{m,i}^{k-1}, \\
\mathfrak{e}_{m,n}^k v_{m,n}^{k+1} + \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{f}_{m,i} v_{i,n}^{k+1} + \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{g}_{n,i} v_{m,i}^{k+1} &= (2 - \mathfrak{e}_{m,n}^k) v_{m,n}^{k-1} + \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{f}_{m,i} v_{i,n}^{k-1} + \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{g}_{n,i} v_{m,i}^{k-1},
\end{aligned} \tag{43}$$

where:

$$\mathfrak{a}_{m,n}^k = 1 - a\tau F(u_{m,n}^k) + \tau G^u(u_{m,n}^k, v_{m,n}^k) + R_1^u g_0^{(\alpha)} + R_2^u g_0^{(\alpha)}, \tag{44}$$

$$\mathfrak{b}_{m,i} = R_1^u g_{m-i}^{(\alpha)}, \tag{45}$$

$$\mathfrak{c}_{n,i} = R_2^u g_{n-i}^{(\alpha)}, \tag{46}$$

$$\mathfrak{e}_{m,n}^k = 1 - \tau c G^v(u_{m,n}^k, v_{m,n}^k) + d\tau + R_1^v g_0^{(\beta)} + R_2^v g_0^{(\beta)}, \tag{47}$$

$$\mathfrak{f}_{m,i} = R_1^v g_{m-i}^{(\beta)}, \tag{48}$$

$$\mathfrak{g}_{n,i} = R_2^v g_{n-i}^{(\beta)}. \tag{49}$$

Let $k \in \bar{I}_K$ and $j \in \bar{I}_M$, and define the $(N+1)$-dimensional vectors:

$$u_j^k = (u_{j,0}^k, u_{j,1}^k, \cdots, u_{j,N-1}^k, u_{j,N}^k)^\top, \tag{50}$$

$$v_j^k = (v_{j,0}^k, v_{j,1}^k, \cdots, v_{j,N-1}^k, v_{j,N}^k)^\top, \tag{51}$$

$$\phi_{u,j}^i = (\phi_{u,j,0}^i, \phi_{u,j,1}^i, \cdots, \phi_{u,j,N-1}^i, \phi_{u,j,N}^i)^\top, \qquad \forall i = 0, 1, \tag{52}$$

$$\phi_{v,j}^i = (\phi_{v,j,0}^i, \phi_{v,j,1}^i, \cdots, \phi_{v,j,N-1}^i, \phi_{v,j,N}^i)^\top, \qquad \forall i = 0, 1. \tag{53}$$

Define then:

$$u^k = u_0^k \oplus u_1^k \oplus \cdots \oplus u_M^k, \tag{54}$$

$$v^k = v_0^k \oplus v_1^k \oplus \cdots \oplus v_M^k, \tag{55}$$

$$\phi_u^0 = \phi_{u,0}^0 \oplus \phi_{u,1}^0 \oplus \cdots \oplus \phi_{u,M}^0, \tag{56}$$

$$\phi_u^1 = \phi_{v,0}^0 \oplus \phi_{v,1}^0 \oplus \cdots \oplus \phi_{v,M}^0, \tag{57}$$

$$\phi_v^0 = \phi_{u,0}^1 \oplus \phi_{u,1}^1 \oplus \cdots \oplus \phi_{u,M}^1, \tag{58}$$

$$\phi_v^1 = \phi_{v,0}^1 \oplus \phi_{v,1}^1 \oplus \cdots \oplus \phi_{v,M}^1. \tag{59}$$

Additionally, define the matrices $B_{m,i}$, C_m^k, $F_{m,i}$, and G_m^k as in Section 3.1, but using now the constants (44)–(49). Next, define the matrices A_u^k and A_v^k through the expressions of A_u^k and A_v^k in (39), using the new constants (44)–(49). On the other hand, we will agree that I is the identity matrix of dimension $(N+1) \times (N+1)$, and set $H_m^k = 2I - C_m^k$ and $J_m^k = 2I - G_m^k$.

Let E_u^k and E_v^k be the block matrices of dimension $(M+1) \times (N+1)$, given by:

$$E_u^k = \begin{pmatrix} H_0^k & -B_{0,1} & \cdots & -B_{0,M} \\ -B_{1,0} & H_1^k & \cdots & -B_{1,M} \\ \vdots & \vdots & \ddots & \vdots \\ -B_{M,0} & -B_{M,1} & \cdots & H_M^k \end{pmatrix}, \quad E_v^k = \begin{pmatrix} J_0^k & -F_{0,1} & \cdots & -F_{0,M} \\ -F_{1,0} & J_1^k & \cdots & -F_{1,M} \\ \vdots & \vdots & \ddots & \vdots \\ -F_{M,0} & -F_{M,1} & \cdots & J_M^k \end{pmatrix}. \tag{60}$$

With this nomenclature, the matrix representation of (43) is given by:

$$\begin{array}{ll} A_u^k u^{k+1} = E_u^k u^{k-1}, & \forall k \in I_{K-1}, \\ A_v^k v^{k+1} = E_v^k v^{k-1}, & \forall k \in I_{K-1}, \\ \text{such that} \begin{cases} u^0 = u_0, \\ u^1 = u_1, \\ v^0 = v_0, \\ v^1 = v_1. \end{cases} & \end{array} \tag{61}$$

4. Structural Properties

The present section is devoted to establishing the main structural properties of the schemes (22) and (43). More precisely, we show the existence and uniqueness of the solutions of both methods. Moreover, we prove that the methods preserve the positive and bounded character of the solutions under appropriate conditions on the parameters.

Definition 7. *A real matrix A is nonnegative if all of its components are nonnegative. In such a case, we use the nomenclature $A \geq 0$. If $\rho \in \mathbb{R}$, then A is said to be bounded from above by ρ if every component of A is at most equal to ρ. This will be denoted by $A \leq \rho$. In the case that $\rho > 0$, then we write $0 \leq A \leq \rho$ to denote that the conditions $A \geq 0$ and $A \leq \rho$ are both satisfied.*

In the following, we will suppose that the functions F, G^u, and G^v are bounded. As a consequence, there exist constants s_1, s_2, and $s_3 \in \mathbb{R}^+$ with the properties that:

$$|F(u_{m,n}^k)| \leq s_1, \qquad |G^u(u_{m,n}^k, v_{m,n}^k)| \leq s_2 \qquad \text{and} \qquad |G^v(u_{m,n}^k, v_{m,n}^k)| \leq s_3, \tag{62}$$

for each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in \bar{I}_K$. Moreover, in the following, we will let $s = \max\{s_1, s_2, s_3\}$. Using these conventions, the following result establishes the main structural properties of the explicit method. It is worth pointing out that the existence and uniqueness of solutions are obviously inherent properties of this scheme in light of its explicit character.

Theorem 1 (Positivity and boundedness)**.** *Let $k \in I_{K-1}$. Assume that F is a bounded function with domain $[0,1]$ and that G^u and G^v are positive and bounded on $[0,1] \times [0,1]$. If $0 \leq u^k \leq 1$, $0 \leq v^k \leq 1$, and:*

$$as\tau + s\tau + R_1^u g_0^{(\alpha)} + R_2^u g_0^{(\alpha)} < 1, \tag{63}$$

$$cs\tau + d\tau + R_1^v g_0^{(\beta)} + R_2^v g_0^{(\beta)} < 1, \tag{64}$$

$$R_1^u \sum_{i=0}^{M} g_{m-i}^{(\alpha)} + R_2^u \sum_{i=0}^{N} g_{n-i}^{(\alpha)} > as\tau, \tag{65}$$

$$d\tau + R_1^v \sum_{i=0}^{M} g_{m-i}^{(\beta)} + R_2^v \sum_{i=0}^{N} g_{n-i}^{(\beta)} > cs\tau, \tag{66}$$

hold, then the solutions of (20) *satisfy $0 \leq u^{k+1} \leq 1$ and $0 \leq v^{k+1} \leq 1$.*

Proof. To prove that $u^{k+1} \geq 0$ and $v^{k+1} \geq 0$, we only need to show that $A_u^k \geq 0$ and $A_v^k \geq 0$. Notice that the off-diagonal elements of A_u^k are equal to $\mathfrak{b}_{m,i}$ (for some $m, i \in \bar{I}_M$ and $i \neq m$) or equal to $\mathfrak{c}_{n,i}$ (for some $n, i \in \bar{I}_N$ and $i \neq n$) or zero. However, $\mathfrak{b}_{m,i} = -R_1^u g_{m-i}^{(\alpha)}$, so Lemma 1(b) assures that $\mathfrak{b}_{m,i} > 0$. Similarly, we can establish that $\mathfrak{c}_{n,i} > 0$. On the other hand, the elements in the diagonal are of the form $a_{m,n}^k$ (for some $m \in \bar{I}_M$ and $n \in \bar{I}_N$). Using (63), one obtains that:

$$\begin{aligned} a_{m,n} &> 1 - a\tau |F(u_{m,n}^k)| - \tau |G^u(u_{m,n}^k, v_{m,n}^k)| - R_1^u g_0^{(\alpha)} - R_2^u g_0^{(\alpha)} \\ &> 1 - as\tau - s\tau - R_1^u g_0^{(\alpha)} - R_2^u g_0^{(\alpha)} > 0. \end{aligned} \tag{67}$$

It follows that $A_u^k \geq 0$, and the proof that A_v^k is established analogously. As a consequence, $u^{k+1} \geq 0$ and $v^{k+1} \geq 0$. To show that the approximations u^k and v^k are bounded, we define the vector $\mathbf{e}$ of dimension $(M+1)(N+1) \times (M+1)(N+1)$ with all elements equal to one. We will prove that $z_u^{k+1} = \mathbf{e} - u^{k+1} > 0$ and that $z_v^{k+1} = \mathbf{e} - v^{k+1} > 0$. Substituting z_u^{k+1} into the first equation of (40), we readily obtain that $z_u^{k+1} = \mathbf{e} - u^{k+1} = \mathbf{e} - A_u^k u^k$, and we only need to show now that $\mathbf{e} - u^{k+1} > 0$. Notice that $\mathbf{e} - u^{k+1}$ is a vector whose components are of the form:

$$y_{m,n} = 1 - \left[\mathfrak{a}_{m,n}^k u_{m,n}^k + \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{b}_{m,i} u_{i,n}^k + \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{c}_{n,i} u_{m,i}^k \right], \tag{68}$$

for $m \in \bar{I}_M$ and $n \in \bar{I}_N$. By hypothesis and (65), we have:

$$\begin{aligned} y_{m,n} &\geq 1 - \left[\mathfrak{a}_{m,n}^k + \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{b}_{m,i} + \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{c}_{n,i} \right] = -a\tau F(u_{m,n}) + \tau G^u(u_{m,n}, v_{m,n}) - \sum_{i=0}^{M} \mathfrak{b}_{m,i} - \sum_{i=0}^{N} \mathfrak{c}_{n,i} \\ &> -as\tau + R_1^u \sum_{i=0}^{M} g_{m-i}^{(\alpha)} + R_2^u \sum_{i=0}^{N} g_{n-i}^{(\alpha)} > 0. \end{aligned} \tag{69}$$

This implies that $z_u^{k+1} > 0$ or, equivalently, that $u^{k+1} \leq 1$. In a similar fashion, we can readily establish the inequality $v^{k+1} \leq 1$. We conclude that $0 \leq u^{k+1} \leq 1$ and $0 \leq v^{k+1} \leq 1$ are satisfied. □

We turn our attention to the structural properties of the scheme (42). To that end, the concept of the Minkowski matrix and its properties will be of utmost importance.

Definition 8. *If all the off-diagonal entries of a real matrix A are non-positive, then A is called a Z-matrix.*

Definition 9. *A real square matrix A is a Minkowski matrix if:*

(i) *A is a Z-matrix,*
(ii) *all the diagonal components of A are positive, and*
(iii) *A is strictly diagonally dominant.*

Minkowski matrices are invertible, and their inverses are positive matrices [45]. This property will be exploited in our results.

Lemma 3. *Let $k \in I_{K-1}$. Suppose that $u^k > 0$ and $v^k > 0$. If $a\tau F(u^k_{m,n}) < 1$, $c\tau G^v(u^k_{m,n}, v^k_{m,n}) < 1$, and $G^u(u^k_{m,n}, v^k_{m,n}) \geq 0$, for each $m \in \bar{I}_M$ and $n \in \bar{I}_N$, then the matrices A^k_u and A^k_v in (39) with the constants (44)–(49) are Minkowski matrices.*

Proof. Clearly, the nonzero off-diagonal elements of A^k_u are equal to $\mathfrak{b}_{m,i}$ (for some $m \in \bar{I}_M$ and $i \neq m$) or $\mathfrak{c}_{n,i}$ (for some $n \in \bar{I}_N$ and $i \neq n$). Notice that $\mathfrak{b}_{m,i} = R^u_1 g^{(\alpha)}_{m-i}$, which means that $\mathfrak{b}_{m,i} < 0$. Similarly, it is easy to see that $\mathfrak{c}_{n,i} < 0$. On the other hand, the entries in the diagonal of A^k_u take the form $\mathfrak{a}^k_{m,n}$ (for $m \in \bar{I}_M$ and $n \in \bar{I}_N$). Lemma 1(a) and the hypotheses show that $\mathfrak{a}^k_{m,n} > 1 - \mathfrak{a}\tau F(u^k_{m,n}) > 0$. The strict diagonal dominance of A^k_u follows from Lemma 1, the hypotheses, and the fact that the following inequalities hold for each $m \in \bar{I}_M$ and each $n \in \bar{I}_N$:

$$\sum_{\substack{i=0\\ i\neq m}}^{M} |\mathfrak{b}_{m,i}| + \sum_{\substack{i=0\\ i\neq n}}^{N} |\mathfrak{c}_{n,i}| = R^u_1 \left[-\sum_{\substack{i=0\\ i\neq m}}^{M} g^{(\alpha)}_{m-i} \right] + R^u_2 \left[-\sum_{\substack{i=0\\ i\neq n}}^{N} g^{(\alpha)}_{n-i} \right] < R^u_1 g^{(\alpha)}_0 + R^u_2 g^{(\alpha)}_0 < a^k_{m,n}. \tag{70}$$

It follows that A^k_u is a Minkowski matrix. That A^k_v is also a Minkowski matrix is proven similarly. □

Theorem 2 (Existence and uniqueness). *Let $k \in I_{K-1}$, and suppose that $u^k > 0$ and $v^k > 0$. If $a\tau F(u^k_{m,n}) < 1$, $c\tau G^v(u^k_{m,n}, v^k_{m,n}) < 1$, and $G^u(u^k_{m,n}, v^k_{m,n}) \geq 0$ for each $m \in \bar{I}_M$ and $n \in \bar{I}_N$, then the recursive system (42) has a unique solution.*

Proof. By hypothesis and Lemma 3, the matrices A^k_u and A^k_v are Minkowski matrices, so nonsingular. It follows that the equations $A^k_u u^{k+1} = E^k_u u^{k-1}$ and $A^k_v v^{k+1} = E^k_v v^{k-1}$ have unique solutions. □

Theorem 3 (Positivity and boundedness). *Let $k \in I_{K-1}$. Suppose that F is a bounded function over $[0,1]$ and that G^u and G^v are positive and bounded on the set $[0,1] \times [0,1]$. If $0 \leq u^k \leq 1$, $0 \leq v^k \leq 1$, and*

$$as\tau + s\tau + R^u_1 g^{(\alpha)}_0 + R^u_2 g^{(\alpha)}_0 < 1, \tag{71}$$

$$cs\tau + d\tau + R^v_1 g^{(\beta)}_0 + R^v_2 g^{(\beta)}_0 < 1, \tag{72}$$

$$R^u_1 \sum_{i=0}^{M} g^{(\alpha)}_{m-i} + R^u_2 \sum_{i=0}^{N} g^{(\alpha)}_{n-i} > as\tau, \tag{73}$$

$$R^v_1 \sum_{i=0}^{M} g^{(\beta)}_{m-i} + R^v_2 \sum_{i=0}^{N} g^{(\beta)}_{n-i} > cs\tau, \tag{74}$$

hold, then the solution of (42) is such that $0 \leq u^{k+1} \leq 1$ and $0 \leq v^{k+1} \leq 1$.

Proof. By hypothesis and Lemma 3, the matrices A^k_u and A^k_v are Minkowski matrices. To show that $u^{k+1} \geq 0$ and $v^{k+1} \geq 0$, use the identities of (61) to obtain:

$$u^{k+1} = (A^k_u)^{-1} E^k_u u^{k-1}, \tag{75}$$

$$v^{k+1} = (A^k_v)^{-1} E^k_v v^{k-1}, \tag{76}$$

where $(A_u^k)^{-1} > 0$ and $(A_v^k)^{-1} > 0$. We need to show now that E_u^k and E_v^k are nonnegative. Note that the off-diagonal elements of E_u^k are either of the form $-\mathfrak{b}_{m,i}$ (with $m, i \in \bar{I}_M$ and $i \neq m$), or $-\mathfrak{c}_{n,i}$ (with $n, i \in \bar{I}_N$ and $i \neq n$), or zeros. As in the proof of Lemma 3, it follows that $\mathfrak{b}_{m,i} < 0$ and $\mathfrak{c}_{n,i} < 0$. Thus, $-\mathfrak{b}_{m,i} > 0$ and $-\mathfrak{c}_{n,i} > 0$. In turn, the elements in the diagonal are of the form $2 - \mathfrak{a}_{m,n}^k$ (for some $m \in \bar{I}_M$ and $n \in \bar{I}_N$). Observe then that (71) implies that:

$$\begin{aligned} 2 - \mathfrak{a}_{m,n}^k &> 1 - a\tau|F(u_{m,n}^k)| - \tau|G^u(u_{m,n}^k, u_{m,n}^k)| - R_1^u g_0^{(\alpha)} - R_2^u g_0^{(\alpha)} \\ &> 1 - as\tau - s\tau - R_1^u g_0^{(\alpha)} - R_2^u g_0^{(\alpha)} > 0. \end{aligned} \tag{77}$$

This shows that $E_u^k > 0$, and we can prove similarly that $E_v^k > 0$. It follows that the approximations u^{k+1} and v^{k+1} are nonnegative, and it only remains to establish the boundedness. Equivalently, we will prove that $z_u^{k+1} = \mathbf{e} - u^{k+1} > 0$ and $z_v^{k+1} = \mathbf{e} - v^{k+1} > 0$. Substituting z_u^{k+1} into (61), we obtain:

$$A_u^k z_u^{k+1} = A_u^k \left(\mathbf{e} - u^{k+1}\right) = A_u^k \mathbf{e} - A_u^k u^{k+1} = A_u^k \mathbf{e} - E_u^k u^{k-1}, \tag{78}$$

where $z_u^{k+1} = (A_u^k)^{-1}(A_u^k \mathbf{e} - E_u^k u^{k-1})$. It suffices to prove that $A_u^k \mathbf{e} - E_u^k u^{k-1} > 0$, but the components of this vector are of the form:

$$y_{m,n} = \mathfrak{a}_{m,n}^k + \sum_{\substack{i=0 \\ i\neq m}}^{M} \mathfrak{b}_{m,i} + \sum_{\substack{i=0 \\ i\neq n}}^{N} \mathfrak{c}_{n,i} - (2 - \mathfrak{a}_{m,n}^k) u_{m,n}^{k-1} + \sum_{\substack{i=0 \\ i\neq m}}^{M} \mathfrak{b}_{m,i} u_{i,n}^{k-1} + \sum_{\substack{i=0 \\ i\neq n}}^{N} \mathfrak{c}_{n,i} u_{m,i}^{k-1}, \tag{79}$$

for $m \in \bar{I}_M$ and $n \in \bar{I}_N$. By hypothesis and (73), it follows that:

$$\begin{aligned} y_{m,n} &\geq \mathfrak{a}_{m,n}^k + \sum_{\substack{i=0 \\ i\neq m}}^{M} \mathfrak{b}_{m,i} + \sum_{\substack{i=0 \\ i\neq n}}^{N} \mathfrak{c}_{n,i} - (2 - \mathfrak{a}_{m,n}^k) u_{m,n}^{k-1} + \sum_{\substack{i=0 \\ i\neq m}}^{M} \mathfrak{b}_{m,i} + \sum_{\substack{i=0 \\ i\neq n}}^{N} \mathfrak{c}_{n,i} \\ &= 2\left[-a\tau F(u_{m,n}^k) + \tau G^u(u_{m,n}^k, v_{m,n}^k) + \sum_{i=0}^{M} \mathfrak{b}_{m,i} + \sum_{i=0}^{N} \mathfrak{c}_{n,i}\right] \\ &> 2\left[-as\tau + R_1^u \sum_{i=0}^{M} g_{m-i}^{(\alpha)} + R_2^u \sum_{i=0}^{N} g_{n-i}^{(\alpha)}\right] > 0. \end{aligned} \tag{80}$$

This implies that $A_u^k \mathbf{e} - E_u^k u^{k-1} > 0$, which means that $z_u^{k+1} > 0$. The proof that $z_v^{k+1} > 0$ can be provided in an entirely analogous way. Finally, we conclude that $0 \leq u^{k+1} \leq 1$ and $0 \leq v^{k+1} \leq 1$. □

5. Numerical Properties

The aim in this section is to prove the most important numerical features of the schemes (20) and (42). For the remainder of this section, we will use the following continuous functionals:

$$\mathcal{L}u(x,t) = \frac{\partial u(x,t)}{\partial t} - auF(u) + uG^u(u,v) - D_1 \sum_{i=1}^{2} \frac{\partial^\alpha u(x,t)}{\partial |x_i|^\alpha}, \qquad \forall (x,t) \in \Omega, \tag{81}$$

$$\mathcal{L}v(x,t) = \frac{\partial v(x,t)}{\partial t} - cvG^v(u,v) + dv - D_2 \sum_{i=1}^{2} \frac{\partial^\beta v(x,t)}{\partial |x_i|^\beta}, \qquad \forall (x,t) \in \Omega. \tag{82}$$

Throughout, we employ the symbol h to represent the vector (h_{x_1}, h_{x_2}).

Definition 10. *We define the infinity norm* $\|\cdot\|_\infty : \mathbb{R}^q \to \mathbb{R}$ *as:*

$$\|v\|_\infty = \max\{|v_i| : i = 1, 2, \ldots, q\}, \qquad \forall v \in \mathbb{R}^q. \tag{83}$$

If E is a real matrix of size $q \times q$, then its infinity norm is given by:

$$\|E\|_\infty = \sup \{\|Ev\|_\infty : v \in \mathbb{R}^q \text{ such that } \|v\|_\infty = 1\} = \max_{1 \le i \le q} \sum_{j=1}^{q} |e_{ij}|. \tag{84}$$

For the remainder, if A is a real square matrix, then $\rho(A)$ will represent its spectral radius.

Lemma 4 (Tian and Huang [46]). *Let $M = (m_{ij})$ be an M-matrix, and let $N = (n_{ij})$ be a nonnegative matrix of the same size as M. If M is strictly diagonally dominant by rows, then $\rho(M^{-1}N)$ satisfies:*

$$\rho(M^{-1}N) \le \max_{i \in N} \left\{ \frac{\sum_{j=1}^{n} n_{ij}}{m_{ii} + \sum_{j \neq i} m_{ij}} \right\}. \tag{85}$$

5.1. Explicit Method

We will establish now the main numerical properties of the scheme (20). To that end, let us introduce the following discrete functionals, for each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$:

$$Lu^k_{m,n} = \delta_t u^k_{m,n} - aF(u^k_{m,n})u^k_{m,n} + G^u(u^k_{m,n}, v^k_{m,n})u^k_{m,n} - D_1 \sum_{i=1}^{2} \delta^{(\alpha)}_{x_i} u^k_{m,n}, \tag{86}$$

$$Lv^k_{m,n} = \delta_t v^k_{m,n} - cG^v(u^k_{m,n}, v^k_{m,n})v^k_{m,n} + dv^k_{m,n} - D_2 \sum_{i=1}^{2} \delta^{(\beta)}_{x_i} v^k_{m,n}. \tag{87}$$

Theorem 4 (Consistency). *Let $u, v \in \mathcal{C}^5(\overline{\Omega}_T)$. If $\tau < 1$, then there are constants $C > 0$ and $C' > 0$ that are independent of τ, h_{x_1}, and h_{x_2}, with the property that for all $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$,*

$$|Lu^k_{m,n} - \mathcal{L}u^k_{m,n}| \le C(\tau + \|h\|^2) \quad \text{and} \quad |Lv^k_{m,n} - \mathcal{L}v^k_{m,n}| \le C'(\tau + \|h\|^2). \tag{88}$$

Proof. We will apply standard arguments using Taylor's theorem and the formula (13) to prove the first inequality of (88). Since $u \in \mathcal{C}^5(\Omega_T)$, there exist constants C_1, $C_{2,i} > 0$ for $i \in \{1, 2\}$ that are independent of τ, h_{x_1}, and h_{x_2}, such that:

$$\left| \delta_t u^k_{m,n} - \frac{\partial u^k_{m,n}}{\partial t} \right| \le C_1 \tau, \tag{89}$$

$$\left| D_i \delta^{(\alpha)}_{x_i} u^k_{m,n} - D_i \frac{\partial^\alpha u^k_{m,n}}{\partial |x_i|^\alpha} \right| \le D_i \left| \delta^{(\alpha)}_{x_i} u^k_{m,n} - \frac{\partial^\alpha u^k_{m,n}}{\partial |x_i|^\alpha} \right| \le C_{2,i} h^2_{x_i}, \tag{90}$$

for each $m \in \bar{I}_M$, $n \in \bar{I}_N$ and $k \in I_{K-1}$. Defining $C = \max\{C_1, C_{2,1}, C_{2,2}\}$ and applying the triangle inequality, we readily check that the first inequality of (88) holds. In a similar fashion, we can also establish the validity of the second inequality. □

Theorem 5 (Nonlinear stability). *Let $(u^k)^K_{k=0}$, $(v^k)^K_{k=0}$ and $(\mathfrak{u}^k)^K_{k=0}$, $(\mathfrak{v}^k)^K_{k=0}$ be two sets of positive and bounded solutions of (20) corresponding to the initial conditions (ϕ^0_u, ϕ^0_v) and $(\phi^0_{\mathfrak{u}}, \phi^0_{\mathfrak{v}})$, respectively. If the matrices A^k_u and $A^k_{\mathfrak{u}}$ are identical to some constant matrix A^k_1 and the matrices A^k_v and $A^k_{\mathfrak{v}}$ are identical to some constant matrix A^k_2 for each $k \in \bar{I}_K$, then there exist constants $C_1, C_2 > 0$ such that:*

$$\|u^k - \mathfrak{u}^k\|_\infty \le C_1 \|u_0 - \mathfrak{u}_0\|_\infty \quad \text{and} \quad \|v^k - \mathfrak{v}^k\|_\infty \le C_2 \|v_0 - \mathfrak{v}_0\|_\infty. \tag{91}$$

Proof. We will only establish the first inequality from (91). Define $\epsilon^k = u^k - \mathfrak{u}^k$, for each $k \in \bar{I}_{K-1}$. By hypothesis, we have that $\epsilon^{k+1} = u^{k+1} - \mathfrak{u}^{k+1} = A_1^k(u^k - \mathfrak{u}^k) = A_1^k \epsilon^k$. Notice that recursion readily shows that $\epsilon^{k+1} = (A_1^k A_1^{k-1} \cdots A_1^1 A_1^0)\epsilon^0$. Taking the infinity norm in both sides, we obtain:

$$\|\epsilon^{k+1}\|_\infty \leq \|A_1^k\|_\infty \|A_1^{k-1}\|_\infty \cdots \|A_1^1\|_\infty \|A_1^0\|_\infty \|\epsilon^0\|_\infty. \tag{92}$$

The conclusion of this result readily follows when we take $C_1 = \|A_1^k\|_\infty \|A_1^{k-1}\|_\infty \cdots \|A_1^1\|_\infty \|A_1^0\|_\infty$. The proof for the second inequality is analogous. □

Theorem 6 (Linear stability). *Let $(u^k)_{k=0}^K$, $(v^k)_{k=0}^K$ be positive and bounded solutions of (20). If the inequalities (63)–(66) hold for each $k \in I_{K-1}$, then the explicit scheme is linearly stable.*

Proof. Using the hypotheses, it is easy to see that for any $m \in \bar{I}_M$ and $n \in \bar{I}_N$,

$$\begin{aligned}
\mathfrak{a}_{m,n}^k + \sum_{\substack{i=0 \\ i\neq m}}^{M} \mathfrak{b}_{m,i} + \sum_{\substack{i=0 \\ i\neq n}}^{N} \mathfrak{c}_{n,i} &\leq 1 + a\tau F(u_{m,n}^k) - R_1^u \sum_{i=0}^{M} g_{m-i}^{(\alpha)} - R_2^u \sum_{i=0}^{N} g_{n-i}^{(\alpha)} \\
&\leq 1 + as\tau - R_1^u \sum_{i=0}^{M} g_{m-i}^{(\alpha)} - R_2^u \sum_{i=0}^{N} g_{n-i}^{(\alpha)} < 1.
\end{aligned} \tag{93}$$

By Lemma 4, we conclude that $\rho(A_u^k) < 1$, and the inequality $\rho(A_v^k) < 1$ is proven in similar fashion. As a consequence, we conclude that the scheme (20) is linearly stable, as desired. □

5.2. Implicit Method

We turn our attention to the theoretical analysis of the scheme (42). Firstly, we establish the accuracy properties of that method. To this end, for each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$, we define the discrete functionals $Lu_{m,n}^k$ and $Lv_{m,n}^k$ as:

$$Lu_{m,n}^k = \delta_t^{(1)} u_{m,n}^k - aF(u_{m,n}^k)\mu_t^{(1)} u_{m,n}^k + G^u(u_{m,n}^k, v_{m,n}^k)\mu_t^{(1)} u_{m,n}^k - D_1 \sum_{i=1}^{2} \mu_t^{(1)} \delta_{x_i}^{(\alpha)} u_{m,n}^k, \tag{94}$$

$$Lv_{m,n}^k = \delta_t^{(1)} v_{m,n}^k - cG^v(u_{m,n}^k, v_{m,n}^k)\mu_t^{(1)} v_{m,n}^k + d\mu_t^{(1)} v_{m,n}^k - D_2 \sum_{i=1}^{2} \mu_t^{(1)} \delta_{x_i}^{(\beta)} v_{m,n}^k. \tag{95}$$

Theorem 7 (Consistency). *Let $u, v \in \mathcal{C}^5(\overline{\Omega}_T)$. If $\tau < 1$, then there exist constants $C > 0$ and $C' > 0$ that are independent of τ, h_{x_1} and h_{x_2} such that for all $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$,*

$$|Lu_{m,n}^k - \mathcal{L}u_{m,n}^k| \leq C(\tau^2 + \|h\|^2) \quad \text{and} \quad |Lv_{m,n}^k - \mathcal{L}v_{m,n}^k| \leq C'(\tau^2 + \|h\|^2). \tag{96}$$

Proof. By the regularity of u, there are constants $C_1, C_2, C_3, C_{4,i} > 0$ for $i = \{1,2\}$, such that:

$$\left| \delta_t^{(1)} u_{m,n}^k - \frac{\partial u_{m,n}^k}{\partial t} \right| \leq C_1 \tau^2, \tag{97}$$

$$\left| aF(u_{m,n}^k)\mu_t^{(1)} u_{m,n}^k - aF(u_{m,n}^k) u_{m,n}^k \right| \leq \left| aF(u_{m,n}^k) \right| \left| \mu_t^{(1)} u_{m,n}^k - u_{m,n}^k \right| \leq C_2 \tau^2, \tag{98}$$

$$\left| G^u(u_{m,n}^k, v_{m,n}^k)\mu_t^{(1)} u_{m,n}^k - G^u(u_{m,n}^k, v_{m,n}^k) u_{m,n}^k \right| \leq \left| G^u(u_{m,n}^k, v_{m,n}^k) \right| \left| \mu_t^{(1)} u_{m,n}^k - u_{m,n}^k \right| \leq C_3 \tau^2, \tag{99}$$

$$\left| D_i \mu_t^{(1)} \delta_{x_i}^{(\alpha)} u_{m,n}^k - D_i \frac{\partial^\alpha u_{m,n}^k}{\partial |x_i|^\alpha} \right| \leq D_i \left| \mu_t^{(1)} \delta_{x_i}^{(\alpha)} u_{m,n}^k - \frac{\partial^\alpha u_{m,n}^k}{\partial |x_i|^\alpha} \right| \leq C_{4,i}(\tau^2 + h_{x_i}^2), \tag{100}$$

for each $m \in \bar{I}_M$, $n \in \bar{I}_N$, and $k \in I_{K-1}$. Let $C = \max\{C_1, C_2, C_3, C_{4,1}, C_{4,2}\}$, and use the triangle inequality to establish the first relation of (96). The proof of the second inequality is analogous. □

Lemma 5 (Chen et al. [47]). *Suppose that A is a matrix of size $m \times m$ and real components, which satisfies:*

$$\sum_{\substack{j=1 \\ j \neq i}}^{m} |a_{ij}| \leq |a_{ii}| - 1, \quad \forall i \in \{1, \ldots, m\}. \tag{101}$$

Then, $\|v\|_\infty \leq \|Av\|_\infty$ is satisfied for all $v \in \mathbb{R}^m$.

Lemma 6. *Let $k \in I_{k-1}$, and suppose that $0 \leq u^k \leq 1$ and $0 \leq v^k \leq 1$. If (73) and (74) are satisfied, then $\|v\|_\infty \leq \|A_u^k v\|_\infty$ and $\|v\|_\infty \leq \|A_v^k v\|_\infty$ hold for all $v \in \mathbb{R}^{(M+1)(N+1)}$.*

Proof. According to Lemma 5, it suffices to show that A_u^k and A_v^k satisfy the inequality (101). Notice that the off-diagonal elements of A_u^k are equal to $\mathfrak{b}_{m,i}$ (for some $m, i \in \bar{I}_M$ and $i \neq m$), or equal to $\mathfrak{c}_{n,i}$ (for some $n, i \in \bar{I}_N$ and $i \neq n$), or zero. On the other hand, the elements in the diagonal are of the form $\mathfrak{a}_{m,n}^k$ (for some $m \in \bar{I}_M$ and $n \in \bar{I}_N$). Using the inequality (73), we observe that:

$$\begin{aligned}
|\mathfrak{a}_{m,n}^k| &= -a\tau F(u_{m,n}^k) + \tau G^u(u_{m,n}^k, v_{m,n}^k) + R_1^u g_0^{(\alpha)} + R_2^u g_0^{(\alpha)} \\
&> -a\tau F(u_{m,n}^k) + R_1^u g_0^{(\alpha)} + R_2^u g_0^{(\alpha)} \\
&> \left[-as\tau + R_1^u \sum_{i=0}^{M} g_{m-i}^{(\alpha)} + R_2^u \sum_{i=0}^{N} g_{n-i}^{(\alpha)} \right] + \sum_{\substack{i=0 \\ i \neq m}}^{M} -R_1^u g_{m-i}^{(\alpha)} + \sum_{\substack{i=0 \\ i \neq n}}^{N} -R_2^u g_{n-i}^{(\alpha)} \\
&> \sum_{\substack{i=0 \\ i \neq m}}^{M} -R_1^u g_{m-i}^{(\alpha)} + \sum_{\substack{i=0 \\ i \neq n}}^{N} -R_2^u g_{n-i}^{(\alpha)} = \sum_{\substack{i=0 \\ i \neq m}}^{M} |\mathfrak{b}_{m,i}| + \sum_{\substack{i=0 \\ i \neq n}}^{N} |\mathfrak{c}_{n,i}|,
\end{aligned} \tag{102}$$

for each $m \in \bar{I}_M$ and each $n \in \bar{I}_N$. Thus, the inequality (101) is satisfied for each row of A_u^k. In a similar fashion, we can prove that the inequality (101) holds for each row of A_v^k. □

Lemma 7. *Let $k \in I_{K-1}$, and suppose that (71)–(74) hold. Then, $E_w^k \geq 0$ and $\|E_w^k\|_\infty < 1$, for $w = u, v$.*

Proof. We have already proven that $E_u^k \geq 0$ in Theorem 3, so we only need to show that $\|E_u^k\|_\infty < 1$. Let $m \in \bar{I}_M$ and $n \in \bar{I}_N$, and observe that the inequality (73) yields:

$$\begin{aligned}
(2 - \mathfrak{a}_{m,n}^k) - \sum_{\substack{i=0 \\ i \neq m}}^{M} \mathfrak{b}_{m,i} - \sum_{\substack{i=0 \\ i \neq n}}^{N} \mathfrak{c}_{n,i} &= 1 + a\tau F(u_{m,n}^k) - \tau G^u(u_{m,n}^k, u_{m,n}^k) - \sum_{i=0}^{M} \mathfrak{b}_{m,i} - \sum_{i=0}^{N} \mathfrak{c}_{n,i} \\
&\leq 1 + a\tau |F(u_{m,n}^k)| - \sum_{i=0}^{M} \mathfrak{b}_{m,i} - \sum_{i=0}^{N} \mathfrak{c}_{n,i} \leq 1 + as\tau - \sum_{i=0}^{M} \mathfrak{b}_{m,i} - \sum_{i=0}^{N} \mathfrak{c}_{n,i} \\
&= 1 - \left[\sum_{i=0}^{M} \mathfrak{b}_{m,i} + \sum_{i=0}^{N} \mathfrak{c}_{n,i} - as\tau \right] < 1.
\end{aligned} \tag{103}$$

Then, the sum of the all elements of each row of the matrix E_u^k is less than one. We conclude that $\|E_u^k\|_\infty < 1$. In a similar way, we can readily establish that $E_v^k \geq 0$ and $\|E_v^k\|_\infty < 1$. □

In our next results, we will establish the nonlinear and the linear stability of the method (42). It is worth pointing out that the study of convergence will be tackled in Theorem 10. An easy variation in the proof of that theorem readily establishes the linear convergence of the explicit scheme.

Theorem 8 (Nonlinear stability). *Let $(u^k)_{k=0}^K$, $(v^k)_{k=0}^K$, and $(\mathfrak{u}^k)_{k=0}^K$, $(\mathfrak{v}^k)_{k=0}^K$ be positive and bounded solutions of (42) corresponding to the initial conditions $(\phi_u^0, \phi_u^1, \phi_v^0, \phi_v^1)$ and $(\phi_\mathfrak{u}^0, \phi_\mathfrak{u}^1, \phi_\mathfrak{v}^0, \phi_\mathfrak{v}^1)$, respectively.*

Suppose that the inequalities (71)–(74) hold for each $k \in \bar{I}_K$. If the matrices $A_1^k = A_u^k = A_{\mathfrak{u}}^k$, $E_1^k = E_u^k = E_{\mathfrak{u}}^k$, $A_2^k = A_v^k = A_{\mathfrak{v}}^k$, and $E_2^k = E_v^k = E_{\mathfrak{v}}^k$ for each $k \in \bar{I}_K$, then:

$$\|u^k - \mathfrak{u}^k\|_\infty \leq \max\{\|u_0 - \mathfrak{u}_0\|_\infty, \|u_1 - \mathfrak{u}_1\|_\infty\}, \tag{104}$$

$$\|v^k - \mathfrak{v}^k\|_\infty \leq \max\{\|v_0 - \mathfrak{v}_0\|_\infty, \|v_1 - \mathfrak{v}_1\|_\infty\}. \tag{105}$$

Proof. Observe that (104) obviously holds if $k \in \{0,1\}$, so assume that it is true for $k \in \{1,\ldots,K-1\}$. Using Lemmas 6 and 7, we have that:

$$\|u^{k+1} - \mathfrak{u}^{k+1}\|_\infty \leq \|A_1^k(u^{k+1} - \mathfrak{u}^{k+1})\|_\infty \leq \|E_1^k(u^{k-1} - \mathfrak{u}^{k-1})\|_\infty \leq \|u^{k-1} - \mathfrak{u}^{k-1}\|_\infty. \tag{106}$$

The conclusion of this result follows now by induction. In an analogous fashion, we may readily show that (105) holds. □

Theorem 9 (Linear stability). *Let $(u^k)_{k=0}^K$, $(v^k)_{k=0}^K$ be positive and bounded solutions of (42). If the inequalities (71)–(74) hold for each $k \in I_{K-1}$, then the scheme (42) is linearly stable.*

Proof. We will use Lemma 4 to prove that $\rho((A_u^k)^{-1}E_u^k) < 1$ and $\rho((A_v^k)^{-1}E_v^k) < 1$. Using the hypotheses, if $m \in \bar{I}_M$ and $n \in \bar{I}_N$, then:

$$\begin{aligned}\frac{(2-\mathfrak{a}_{m,n}^k) - \sum\limits_{\substack{i=0\\ i\neq m}}^{M}\mathfrak{b}_{m,i} - \sum\limits_{\substack{i=0\\ i\neq n}}^{N}\mathfrak{c}_{n,i}}{\mathfrak{a}_{m,n}^k + \sum\limits_{\substack{i=0\\ i\neq m}}^{M}\mathfrak{b}_{m,i} + \sum\limits_{\substack{i=0\\ i\neq n}}^{N}\mathfrak{c}_{n,i}} &\leq \frac{1 + a\tau F(u_{m,n}^k) - R_1^u\sum\limits_{i=0}^{M} g_{m-i}^{(\alpha)} - R_2^u\sum\limits_{i=0}^{N} g_{n-i}^{(\alpha)}}{1 - a\tau F(u_{m,n}^k) + R_1^u\sum\limits_{i=0}^{M} g_{m-i}^{(\alpha)} + R_2^u\sum\limits_{i=0}^{N} g_{n-i}^{(\alpha)}}\\ &\leq \frac{1 + as\tau - R_1^u\sum\limits_{i=0}^{M} g_{m-i}^{(\alpha)} - R_2^u\sum\limits_{i=0}^{N} g_{n-i}^{(\alpha)}}{1 - as\tau + R_1^u\sum\limits_{i=0}^{M} g_{m-i}^{(\alpha)} + R_2^u\sum\limits_{i=0}^{N} g_{n-i}^{(\alpha)}} < 1.\end{aligned} \tag{107}$$

Notice that $\rho((A_u^k)^{-1}E_u^k) < 1$ holds since every quotient is less than one. In a similar fashion, we can readily prove that $\rho((A_v^k)^{-1}E_v^k) < 1$. As a consequence, we conclude that (42) is linearly stable. □

Theorem 10 (Convergence). *Suppose that $\mathfrak{u}, \mathfrak{v} \in \mathcal{C}^5(\overline{\Omega}_T)$ are positive and bounded solutions of (14). Let $\tau < 1$, and suppose that $(u^k)_{k=0}^K$ and $(v^k)_{k=0}^K$ are positive and bounded solutions of (43). If (71)–(74) are satisfied for all $k \in \bar{I}_K$, then there are constants $\kappa_u, \kappa_v \in \mathbb{R}^+$ that are independent of τ and h, such that:*

$$\|\mathfrak{u}^k - u^k\|_\infty \leq \kappa_u(\tau^2 + \|h\|^2), \quad \forall k \in \bar{I}_K, \tag{108}$$

$$\|\mathfrak{v}^k - v^k\|_\infty \leq \kappa_v(\tau^2 + \|h\|^2), \quad \forall k \in \bar{I}_K. \tag{109}$$

Proof. Define $\epsilon^k = \mathfrak{u}^k - u^k$, for each $k \in \bar{I}_K$. Since the exact and the numerical solutions coincide on the initial data, then $\|\epsilon^0\|_\infty = \|\epsilon^1\|_\infty = 0$. Using Theorem 7 and Lemmas 6 and 7, we obtain:

$$\begin{aligned}\|\epsilon^{k+1}\|_\infty &\leq \|A_u(\mathfrak{u}^{k+1} - u^{k+1})\|_\infty \leq \|E_u(\mathfrak{u}^{k-1} - u^{k-1})\|_\infty + \|A\mathfrak{u}^{k+1} - E\mathfrak{u}^{k-1}\|_\infty\\ &= \|\epsilon^{k-1}\|_\infty + \tau\|L\mathfrak{u}^k - \mathcal{L}\mathfrak{u}^k\|_\infty \leq \|\epsilon^{k-1}\|_\infty + \tau C(\tau^2 + \|h\|^2),\end{aligned} \tag{110}$$

which yields that $\|\epsilon^{k+1}\|_\infty - \|\epsilon^{k-1}\|_\infty \leq \tau C(\tau^2 + \|h\|^2)$ for all $k \in I_{K-1}$. The conclusion follows now if we let $\kappa_u = TC$. In a similar way, we can prove that there exists a constant κ_v satisfying (109). As a conclusion, the scheme (43) is quadratically convergent. □

6. Applications

The present section will be devoted to providing some computer simulations to illustrate the applicability of the finite difference schemes proposed in this work. In the first stage, we must point out that the explicit scheme (20) is obviously more suitable than the implicit model (42) when investigating two- and three-dimensional regimes [48,49]. To implement it efficiently, we notice firstly that the first equation of (20) can be rewritten as:

$$u_{m,n}^{k+1} = u_{m,n}^k + \tau W(u_{m,n}^k, v_{m,n}^k) + \tau D_1 \sum_{i=1}^{2} \delta_{x_i}^{(\alpha)} u_{m,n}^k, \tag{111}$$

where:

$$W(u_{m,n}^k, v_{m,n}^k) = aF(u_{m,n}^k)u_{m,n}^k - G^u(u_{m,n}^k, v_{m,n}^k)u_{m,n}^k, \tag{112}$$

for each $m \in \overline{I}_M$, $n \in \overline{I}_N$, and $k \in \overline{I}_{K-1}$. Let W be the real matrix of size $(M+1) \times (N+1)$ whose entry at the row $m \in \overline{I}_M$ and column $n \in \overline{I}_N$ is $W_{m,n} = W(u_{m,n}^k, v_{m,n}^k)$. Similarly, U^k will represent the matrix of the same size as W such that $U_{m,n}^k = u_{m,n}^k$.

Notice now that:

$$\delta_{x_1}^{(\alpha)} u_{m,n}^k = -\frac{1}{h_{x_1}^\alpha} \sum_{i=0}^{M} g_{m-i}^{(\alpha)} u_{i,n}^k = -\frac{1}{h_{x_1}} \left[H_M^{(\alpha)} * U^k \right]_{m,n}, \tag{113}$$

$$\delta_{x_2}^{(\alpha)} u_{m,n}^k = -\frac{1}{h_{x_2}^\alpha} \sum_{i=0}^{N} u_{m,i}^k g_{n-i}^{(\alpha)} = -\frac{1}{h_{x_2}} \left[U^k * H_N^{(\alpha)} \right]_{m,n}. \tag{114}$$

Here, $*$ represents the usual operation of matrix multiplication, and for each $q \in \mathbb{N}$, $H_q^{(\alpha)}$ represents the real symmetric matrix of size $(q+1) \times (q+1)$ defined by:

$$H_q^{(\alpha)} = \begin{pmatrix} g_0^{(\alpha)} & g_1^{(\alpha)} & g_2^{(\alpha)} & \cdots & g_q^{(\alpha)} \\ g_1^{(\alpha)} & g_0^{(\alpha)} & g_1^{(\alpha)} & \cdots & g_{q-1}^{(\alpha)} \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & \cdots & g_{q-2}^{(\alpha)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ g_q^{(\alpha)} & g_{q-1}^{(\alpha)} & g_{q-2}^{(\alpha)} & \cdots & g_0^{(\alpha)} \end{pmatrix}. \tag{115}$$

From this, it is easy to see now that the set of equations (111) can be rewritten equivalently in matrix form as $U^{k+1} = U^k + \tau W - R_1^u H_M^{(\alpha)} * U^k - R_2^u U^k H_N^{(\alpha)}$.

Summarizing, the explicit scheme (20) can be expressed alternatively in matrix form as:

$$\begin{aligned} &U^{k+1} = U^k + \tau W - R_1^u H_M^{(\alpha)} * U^k - R_2^u U^k H_N^{(\alpha)}, \\ &V^{k+1} = V^k + \tau Z - R_1^v H_M^{(\beta)} * V^k - R_2^v V^k H_N^{(\beta)}, \\ &\text{such that } \begin{cases} U^0 = \Phi^u, \\ V^0 = \Phi^v. \end{cases} \end{aligned} \tag{116}$$

In this formula, we convey that $\Phi_{m,n}^u = \phi_{u,m,n}^0$ and $\Phi_{m,n}^v = \phi_{v,m,n}^0$, for each $(m,n) \in \overline{I}_M \times \overline{I}_N$. Moreover, we let Z be the real matrix of size $(M+1) \times (N+1)$ whose entry at the position $(m,n) \in \overline{I}_M \times \overline{I}_N$ is defined by $Z(u_{m,n}^k, v_{m,n}^k)$, where:

$$Z(u_{m,n}^k, v_{m,n}^k) = cG^v(u_{m,n}^k, v_{m,n}^k)v_{m,n}^k - dv_{m,n}^k. \tag{117}$$

Likewise, V^k denotes the matrix of the same size as X with the property that $V_{m,n}^k = v_{m,n}^k$, for each $(m,n) \in \overline{I}_M \times \overline{I}_N$ and $k \in \overline{I}_K$. For the sake of convenience, we have included a MATLAB implementation of the scheme (116) in the Appendix. It is worth pointing out that the scheme is actually very general, not only in the sense that it accounts for different fractional differentiation orders, but also because the functions W and X therein are arbitrary.

The following examples will make use of variants of the MATLAB code provided in Appendix A. For the sake of illustration, the models considered will be in two spatial dimensions.

Example 1. *In this example, we let $\Omega = (0, 100) \times (0, 100)$ and $T = 3000$. Throughout, we will consider the following diffusion-reaction system, defined for each $(x, t) \in \Omega$:*

$$\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= au(x,t)\left[1 - u(x,t)\right] - \frac{u(x,t)v(x,t)}{u(x,t)+v(x,t)} + D_1\left(\frac{\partial^\alpha u(x,t)}{\partial |x_1|^\alpha} + \frac{\partial^\alpha u(x,t)}{\partial |x_2|^\alpha}\right), \\
\frac{\partial v(x,t)}{\partial t} &= \frac{cu(x,t)v(x,t)}{u(x,t)+v(x,t)} - dv(x,t) + D_2\left(\frac{\partial^\beta u(x,t)}{\partial |x_1|^\beta} + \frac{\partial^\beta u(x,t)}{\partial |x_2|^\beta}\right).
\end{aligned} \tag{118}$$

Here, the constants a, c, d, D_1, and D_2 are positive, and we will define:

$$(u^*, v^*) = \left(\frac{ac - c + d}{ac}, \frac{(c-d)(ac - c + d)}{acd}\right) \in \mathbb{R}^2. \tag{119}$$

It is easy to see that this point is a stationary solution of (118), which is a model that describes the spatio-temporal dynamics of a predator–prey system without Allee effects. Obviously, this system is a particular form of the more general model (7). To approximate solutions of the present system of equations, we will let $\phi_v(x)$ be any sample from a normally distributed random variable with the mean equal to v^* and the standard deviation equal to 0.01. Meanwhile, ϕ_u will be equal to zero on all B, except on a central square at the middle of B, on which it will be constantly equal to 0.2. Let $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, and $D_2 = 0.6$. Figure 1 provides snapshots of the solution u in (118) at (a) $t = 0$, (b) $t = 160$, (c) $t = 290$, (d) $t = 500$, (e) $t = 1010$, and (f) $t = 3000$, using $\alpha = \beta = 2$. The graphs exhibit the presence of complex patterns, in agreement with the results obtained in [43]. In those results, we agreed that $x = x_1$ and $y = x_2$. For illustration purposes, Figures 2 and 3 provide similar results for the cases when $\alpha = \beta = 1.6$ and $\alpha = \beta = 1.2$, respectively. Turing patterns appear in those instances also, in spite of the fractional nature of those cases. In our simulations, we used our implementation of (20) shown in Appendix A, with $\tau = 0.02$ and $h_{x_1} = h_{x_2} = 1/3$. Moreover, we imposed homogeneous Neumann conditions on the boundary of B.

It is worth pointing out that the literature lacks an analytical apparatus that justifies the presence of the Turing patterns in the fractional scenarios of Figures 2 and 3. In that sense, the explicit numerical methodology reported in the present paper may be a reliable tool to confirm any analytical results on the fully fractional form of (118).

In our last example, we will tackle the three-dimensional scenario. To that end, the code of Appendix A had to be adapted to the three-dimensional scenario, and parallel programming was needed in order to speed up the computer time.

Example 2. *We considered the three-dimensional form of problem (118) with the same model parameters, spatial domain $\Omega = (0, 100) \times (0, 100) \times (0, 100) \subseteq \mathbb{R}^3$, $\tau = 0.02$, and $h_{x_1} = h_{x_2} = h_{x_3} = 1$. Under these circumstances, Figure 4 shows snapshots of the solution u of the three-dimensional problem (118) at (a) $t = 0$, (b) $t = 160$, (c) $t = 290$, (d) $t = 500$, (e) $t = 1010$, and (f) $t = 3000$, letting $\alpha = \beta = 1.6$. The graphs exhibit the presence of complex three-dimensional patterns that have not been investigated in the literature. For convenience, Figure 5 shows x-, y- and z-cross sections of the approximate solution u at the same times. In this case, the graphs exhibit the presence of two-dimensional patterns on the sides of the cube $\overline{B}$. In turn, Figures 6 and 7 show similar results for the case when $\alpha = \beta = 1.2$. Again, the presence of three-dimensional and two-dimensional patterns is obvious from the graphs. We performed more simulations (not included in this work to avoid redundancy) using various values of α and β. The results have shown the presence of three-dimensional complex patterns in all the cases considered.*

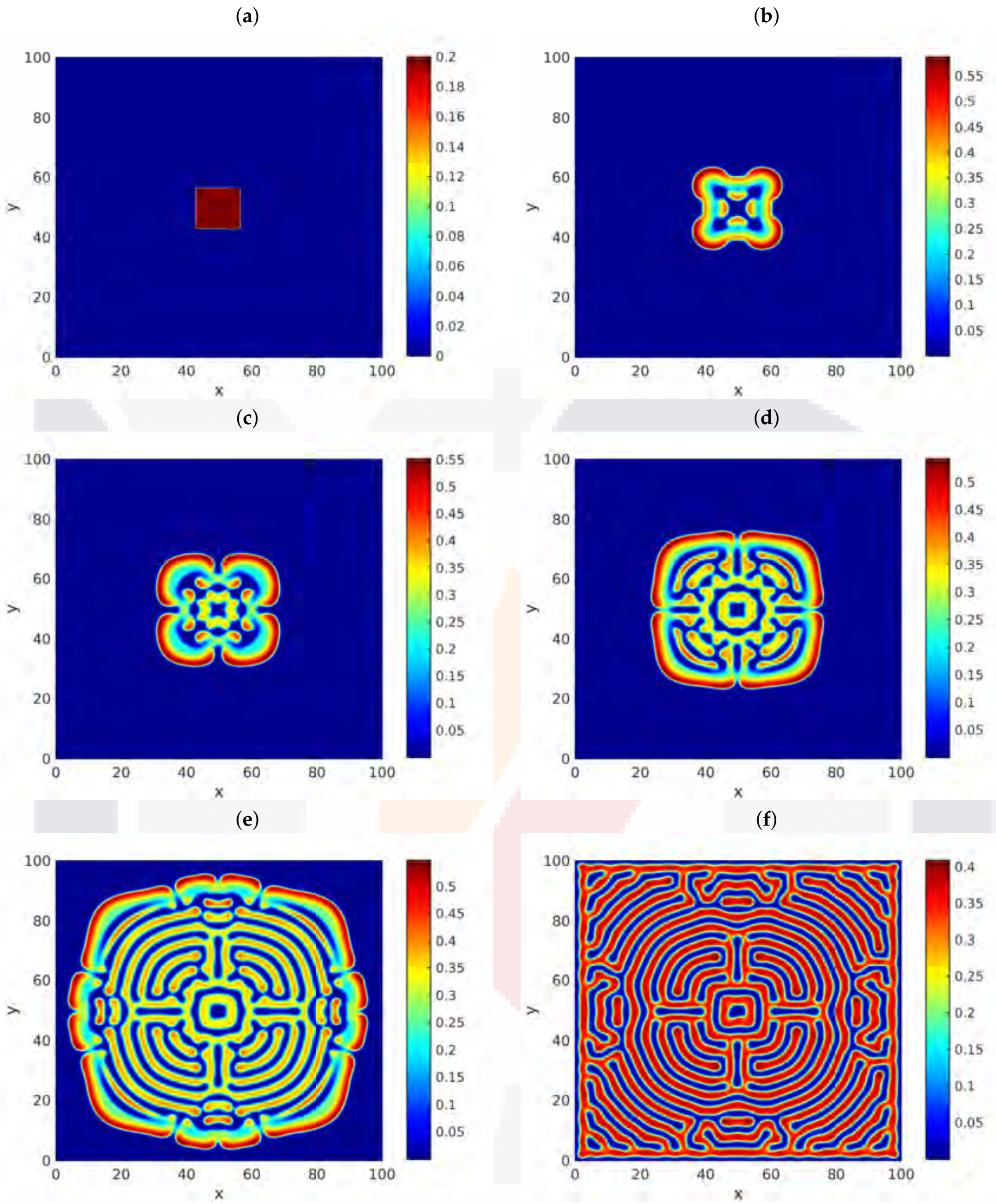

Figure 1. Snapshots of the approximate solution u in (118) versus x and y. The parameters employed are $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, and $\alpha = \beta = 2$. Meanwhile, we considered the times (**a**) $t = 0$, (**b**) $t = 160$, (**c**) $t = 290$, (**d**) $t = 500$, (**e**) $t = 1010$, and (**f**) $t = 3000$. We let $\phi_v(x)$ be a random sample from a normally distributed random variable with the mean equal to v^* and the standard deviation equal to 0.01, and ϕ_u is the function depicted in (a). The approximations were calculated using our implementation of (20) shown in Appendix A, with $\tau = 0.02$ and $h_{x_1} = h_{x_2} = 1/3$.

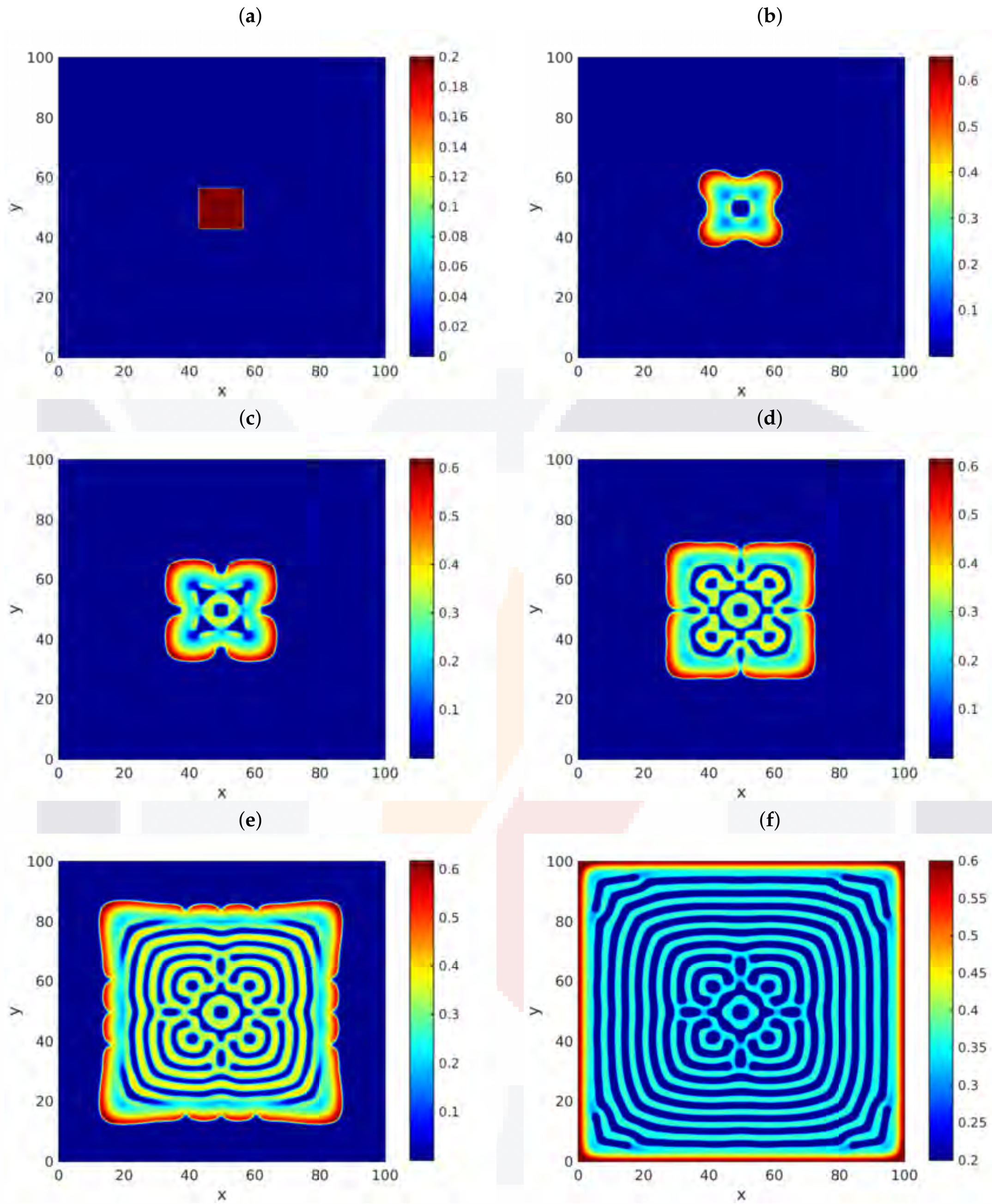

Figure 2. Snapshots of the approximate solution u in (118) versus x and y. The parameters employed are $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, and $\alpha = \beta = 1.6$. Meanwhile, we considered the times (**a**) $t = 0$, (**b**) $t = 160$, (**c**) $t = 290$, (**d**) $t = 500$, (**e**) $t = 1010$, and (**f**) $t = 3000$. We let $\phi_v(x)$ be a random sample from a normally distributed random variable with the mean equal to v^* and the standard deviation equal to 0.01, and ϕ_u is the function depicted in (a). The approximations were calculated using our implementation of (20) shown in Appendix A, with $\tau = 0.02$ and $h_{x_1} = h_{x_2} = 1/3$.

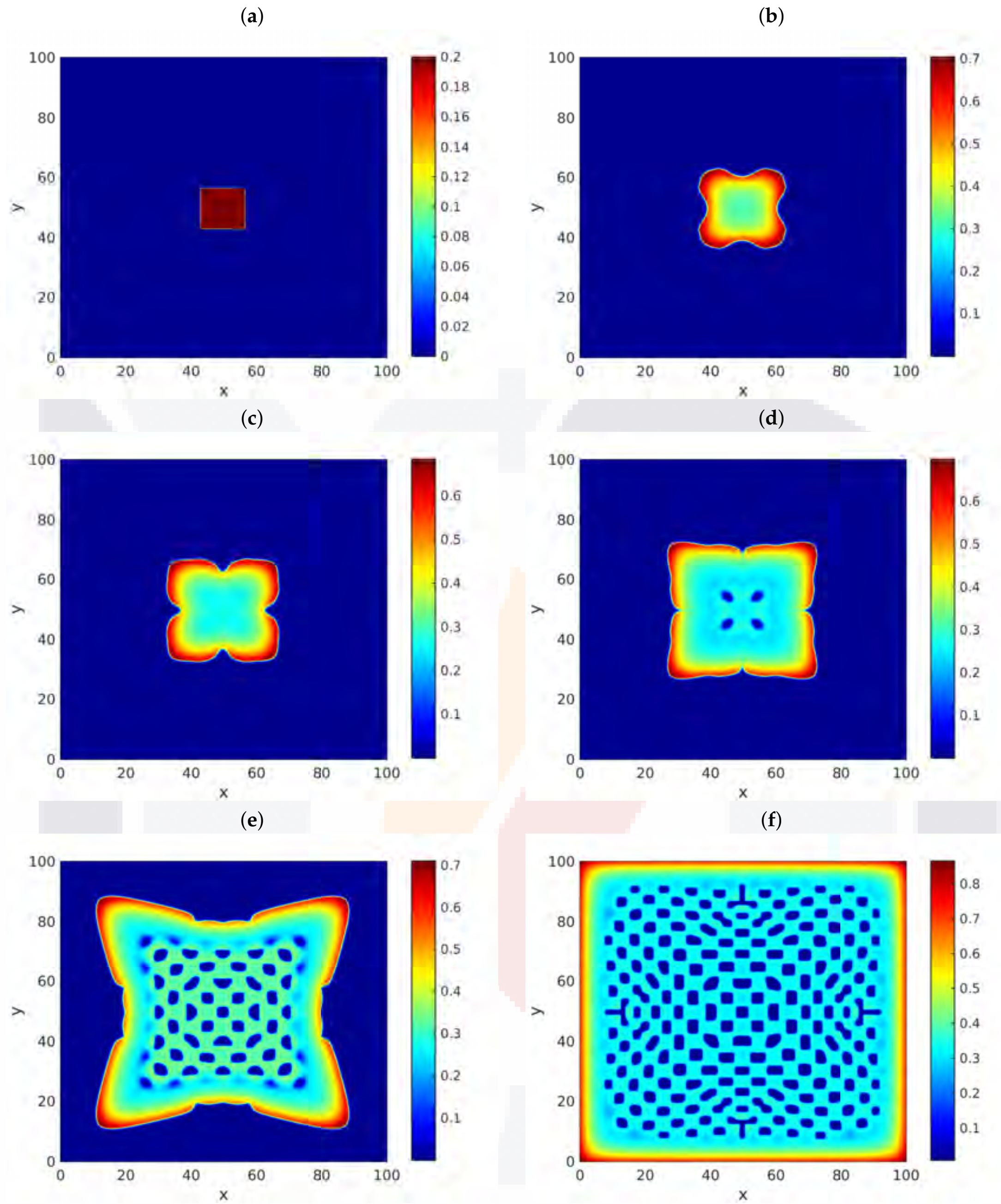

Figure 3. Snapshots of the approximate solution u in (118) versus x and y. The parameters employed are $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, and $\alpha = \beta = 1.2$. Meanwhile, we considered the times (**a**) $t = 0$, (**b**) $t = 160$, (**c**) $t = 290$, (**d**) $t = 500$, (**e**) $t = 1010$, and (**f**) $t = 3000$. We let $\phi_v(x)$ be a random sample from a normally distributed random variable with the mean equal to v^* and the standard deviation equal to 0.01, and ϕ_u is the function depicted in (a). The approximations were calculated using our implementation of (20) shown in Appendix A, with $\tau = 0.02$ and $h_{x_1} = h_{x_2} = 1/3$.

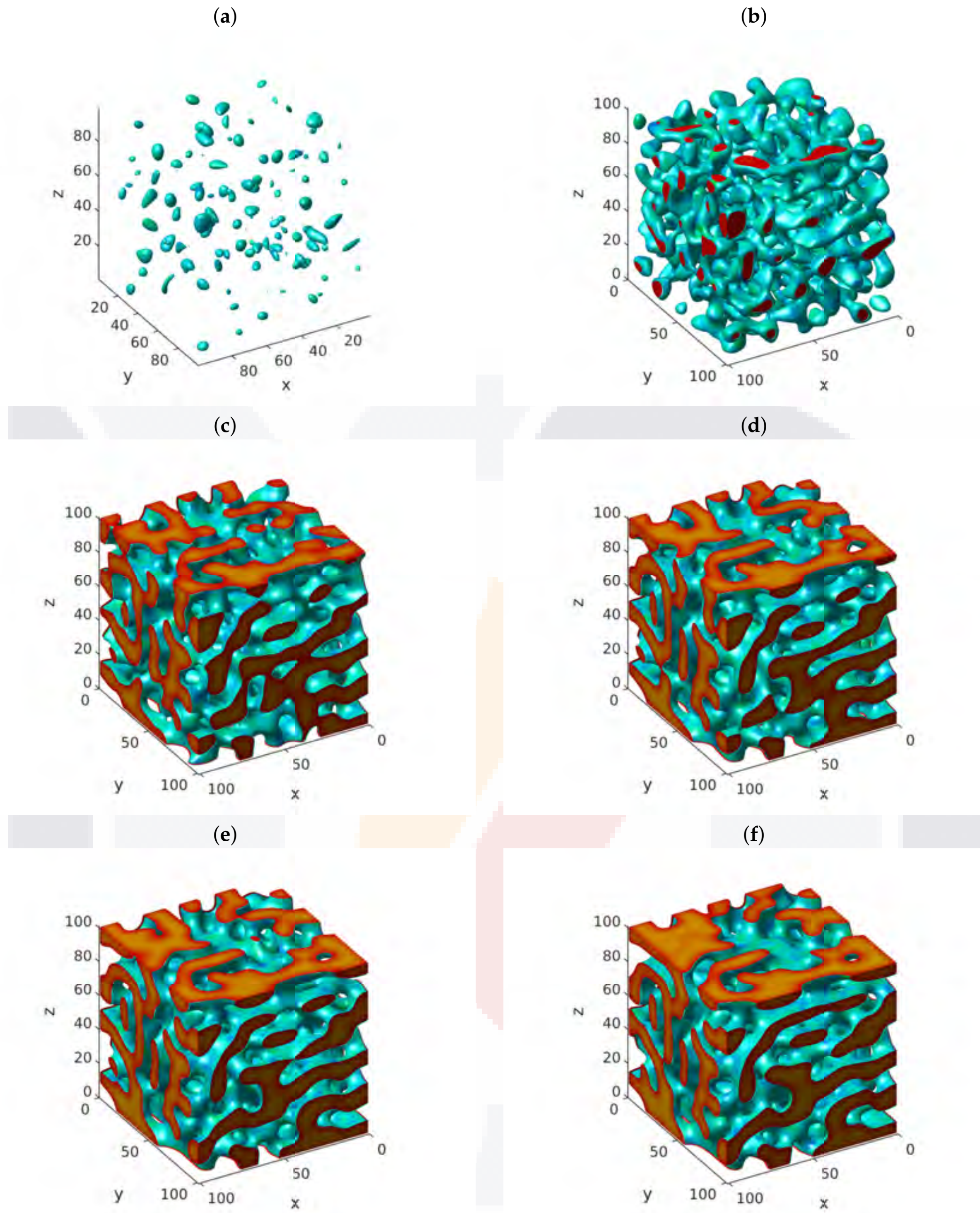

Figure 4. Snapshots of the approximate solution u in (118) versus x, y, and z. The parameters employed are $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, and $\alpha = \beta = 1.6$. Meanwhile, we considered the times (**a**) $t = 0$, (**b**) $t = 160$, (**c**) $t = 290$, (**d**) $t = 500$, (**e**) $t = 1010$, and (**f**) $t = 3000$. The initial data are random samples of a uniform distribution on $[0, 1]$. The approximations were calculated using our implementation of (20), with $\tau = 0.02$ and $h_{x_1} = h_{x_2} = h_{x_3} = 1$.

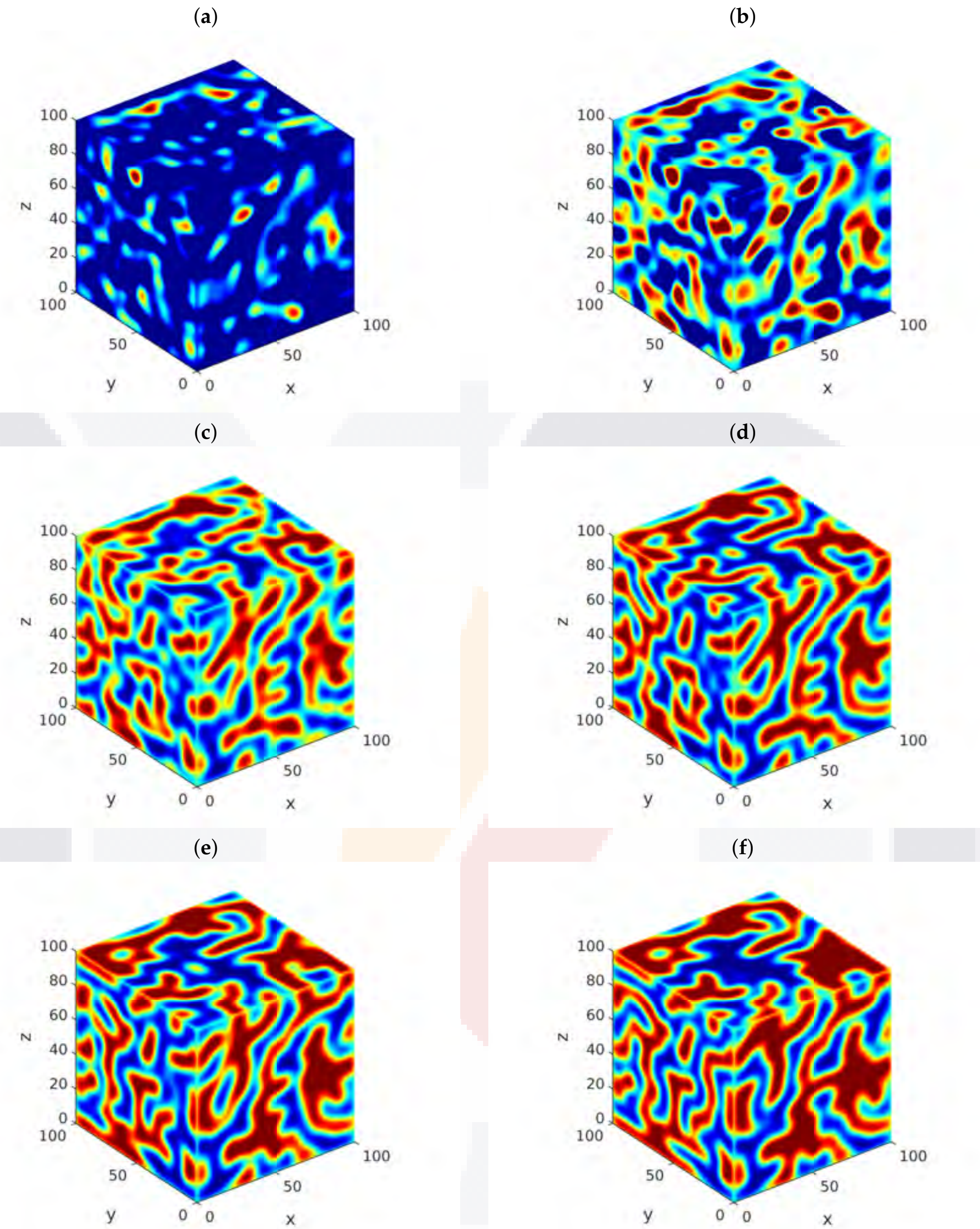

Figure 5. Snapshots of x-, y-, and z-cross-sections of the approximate solution u of (118) versus x, y, and z. The parameters employed are $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, and $\alpha = \beta = 1.6$. Meanwhile, we considered the times (**a**) $t = 0$, (**b**) $t = 160$, (**c**) $t = 290$, (**d**) $t = 500$, (**e**) $t = 1010$, and (**f**) $t = 3000$. The initial data are random samples of a uniform distribution on $[0, 1]$. The approximations were calculated using our implementation of (20), with $\tau = 0.02$ and $h_{x_1} = h_{x_2} = h_{x_3} = 1$.

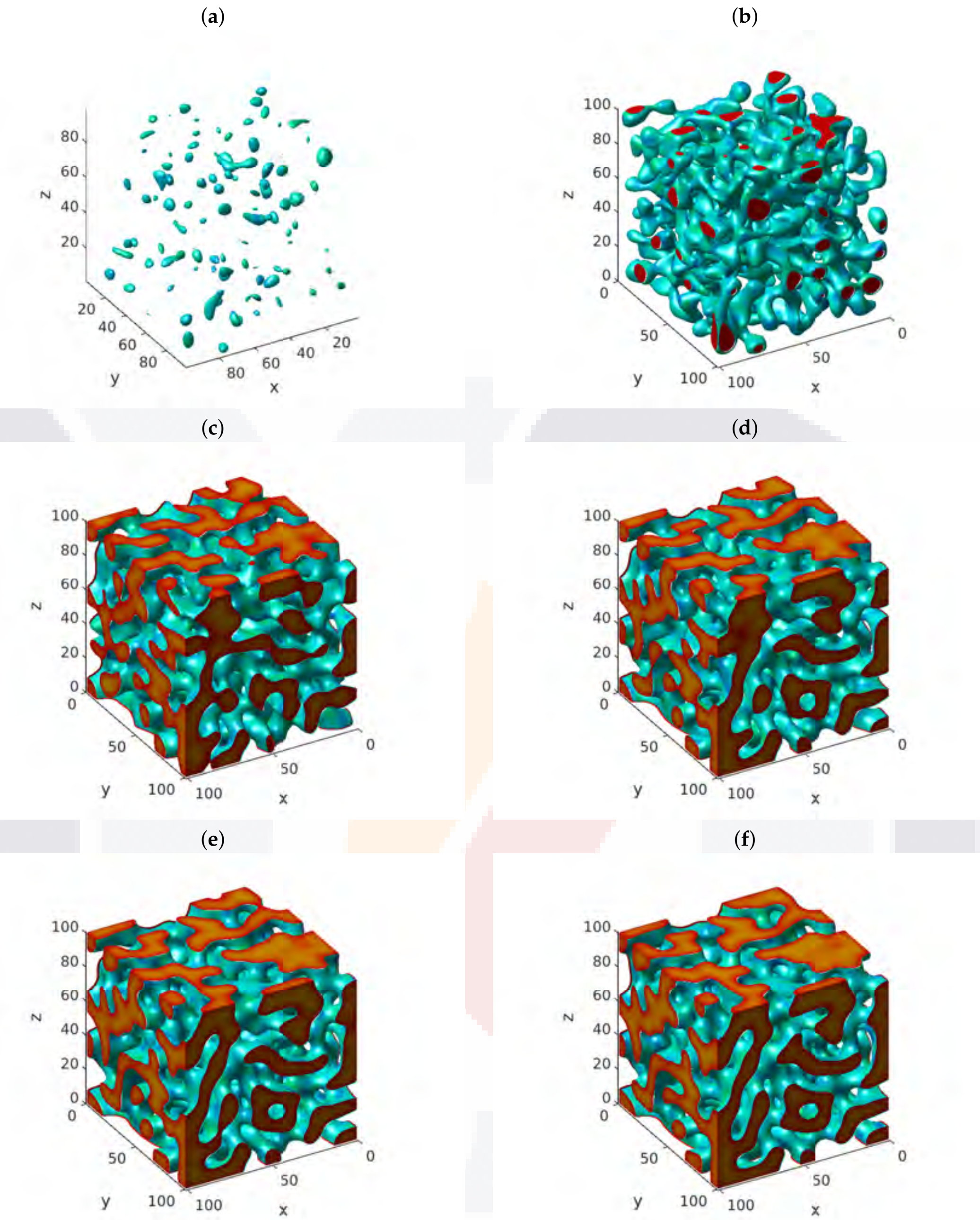

Figure 6. Snapshots of the approximate solution u of (118) versus x, y, and z. The parameters employed are $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, and $\alpha = \beta = 1.2$. Meanwhile, we considered the times (**a**) $t = 0$, (**b**) $t = 160$, (**c**) $t = 290$, (**d**) $t = 500$, (**e**) $t = 1010$, and (**f**) $t = 3000$. The initial data are random samples of a uniform distribution on $[0, 1]$. The approximations were calculated using our implementation of (20), with $\tau = 0.02$ and $h_{x_1} = h_{x_2} = h_{x_3} = 1$.

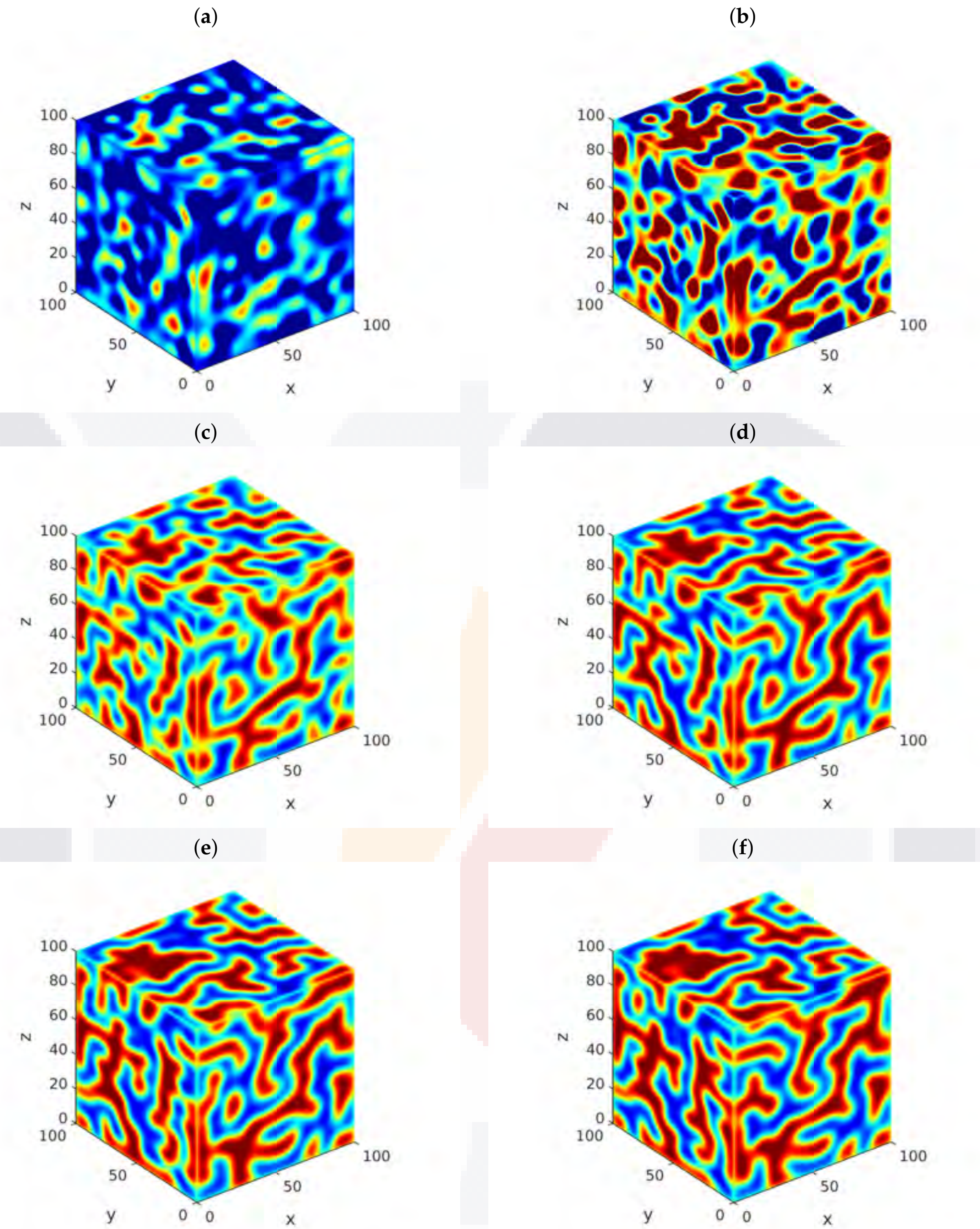

Figure 7. Snapshots of x-, y-, and z-cross-sections of the approximate solution u of (118) versus x, y, and z. The parameters employed are $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, and $\alpha = \beta = 1.2$. Meanwhile, we considered the times (**a**) $t = 0$, (**b**) $t = 160$, (**c**) $t = 290$, (**d**) $t = 500$, (**e**) $t = 1010$, and (**f**) $t = 3000$. The initial data are random samples of a uniform distribution on $[0, 1]$. The approximations were calculated using our implementation of (20), with $\tau = 0.02$ and $h_{x_1} = h_{x_2} = h_{x_3} = 1$.

Our last example provides numerical evidence that the emerging Turing patterns preserve their share independent of the discretization step.

Example 3. *Consider the same mathematical problem of Example 1 with the model parameters* $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, *and* $\alpha = \beta = 1.6$. *Fix the temporal period* $T = 500$. *Figure 8 shows the results of our simulations considering various values of the spatial partition norms. Throughout, we let* $h = h_{x_1} = h_{x_2}$.

The graphs correspond to the values (a) $h = 1/3$, (b) $h = 1/4$, $h = 1/5$, and $h = 1/8$. A similar pattern shape was obtained in all cases. These results provide numerical evidence that the type of Turing pattern is independent of the discretization spatial step-size. We performed similar experiments considering different temporal steps. The simulations are not reproduced to avoid redundancy, but they prove that the emerging patterns are also independent of τ.

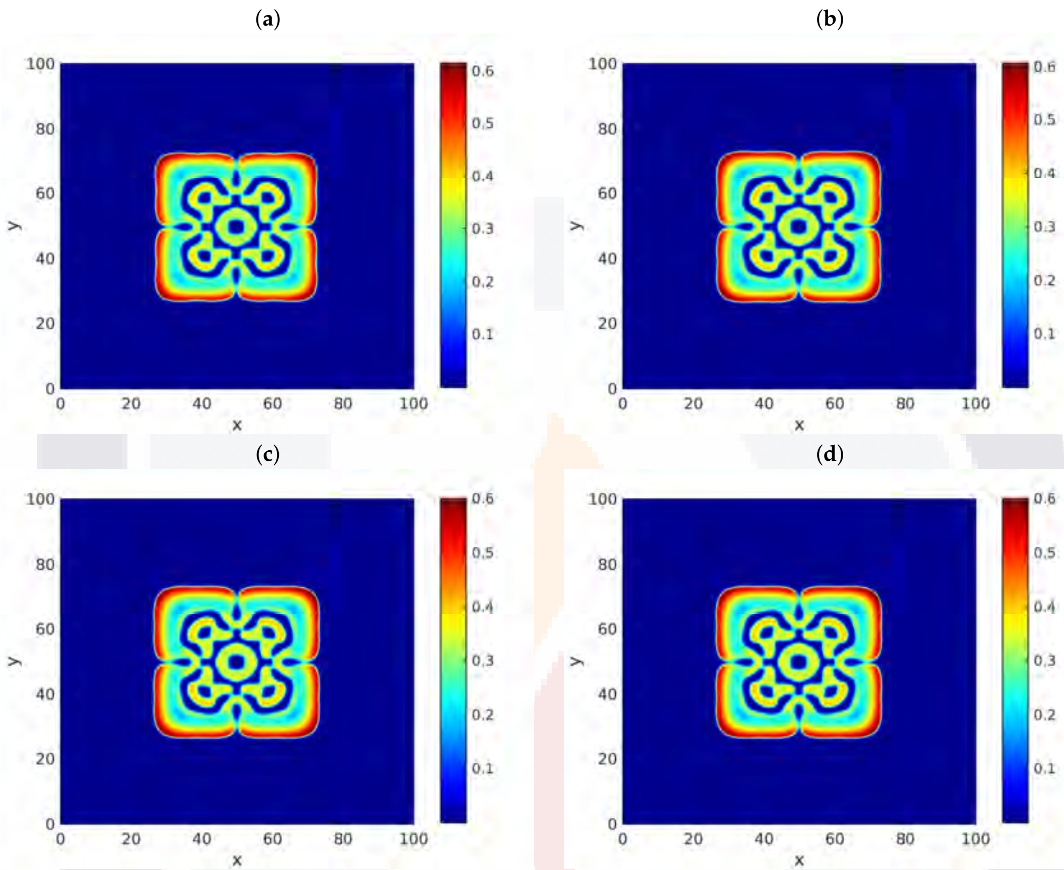

Figure 8. Snapshots of the approximate solution u in (118) versus x and y, at the time $T = 500$. The parameters employed are $a = 0.8$, $c = 0.3$, $d = 0.1$, $D_1 = 0.01$, $D_2 = 0.6$, and $\alpha = \beta = 1.6$. We let $\phi_v(x)$ be a random sample from a normally distributed random variable with the mean equal to v^* and the standard deviation equal to 0.01, and ϕ_u is the function depicted in (**a**). The approximations were calculated using our implementation of (20) shown in Appendix A, with $\tau = 0.02$ and $h = h_{x_1} = h_{x_2}$ satisfying (**a**) $h = 1/3$, (**b**) $h = 1/4$, (**c**) $h = 1/5$, and (**d**) $h = 1/8$.

7. Conclusions

In this manuscript, we studied computationally a system of two diffusive partial differential equations with coupled nonlinear reactions in generalized forms. Our system considered the presence of anomalous diffusion in multiple spatial dimensions along with suitable initial data. The model generalized various particular systems from the physical sciences, including the diffusive systems, which describe the interaction between populations of predators and preys with the Michaelis–Menten-type reaction. The system was discretized following a finite-difference approach, and two schemes were proposed to approximate the solutions. The two numerical models were rigorously analyzed to elucidate their structural and numerical properties.

As the main structural results, we established the existence and uniqueness of the numerical solutions. Moreover, we proved that the schemes were both capable of preserving the positivity and boundedness of approximations [50,51]. As in various other examples available in the literature [31,52–54], this was in perfect agreement with the fact that the relevant solutions of normalized population models were positive and bounded. Numerically, we proved rigorously that the schemes were consistent, stable, and convergent. Some simulations were provided in this work to illustrate the performance of the schemes. In particular, we showed the capability of one of the schemes to be applied on the investigation of Turing patterns in anomalously diffusive systems describing predator–prey interactions. To that end, a fast computational implementation in MATLAB of one of the schemes was employed. Of course, the present approach may be applied to other different scenarios [55,56].

At the closure of this manuscript, it is interesting to point out that the two discretizations of the system (7) were capable of preserving the anomalous diffusion rate. Indeed, note that those rates were equal to D_1 and D_2 for each of the partial differential equations of the continuous model (7). On the other hand, in light of Lemma 2, it follows that:

$$\begin{aligned} D_1 \sum_{i=1}^{2} \delta_{x_i}^{(\alpha)} u_{m,n}^k &= D_1 \left[-\frac{1}{h_{x_1}^\alpha} \sum_{i=0}^{M} g_{m-i}^{(\alpha)} u_{i,n}^k - \frac{1}{h_{x_2}^\alpha} \sum_{i=0}^{N} g_{n-i}^{(\alpha)} u_{m,i}^k \right] \\ &= D_1 \left[\frac{\partial^\alpha u(x_{1,m}, x_{2,n}, t_k)}{\partial |x_1|^\alpha} + \frac{\partial^\alpha u(x_{1,m}, x_{2,n}, t_k)}{\partial |x_2|^\alpha} \right] + \mathcal{O}(h_{x_1}^2) + \mathcal{O}(h_{x_2}^2) \\ &= D_1 \sum_{i=1}^{2} \frac{\partial^\alpha u(x_{1,m}, x_{2,n}, t_k)}{\partial |x_i|^\alpha} + \mathcal{O}(\|h\|^2). \end{aligned} \tag{120}$$

Similarly, it is easy to check that:

$$D_2 \sum_{i=1}^{2} \delta_{x_i}^{(\beta)} v_{m,n}^k = D_2 \sum_{i=1}^{2} \frac{\partial^\beta v(x_{1,m}, x_{2,n}, t_k)}{\partial |x_i|^\beta} + \mathcal{O}(\|h\|^2). \tag{121}$$

It follows that our spatial discretizations are capable of preserving the anomalous diffusion rate.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. MATLAB Code

The following is a basic implementation in MATLAB of the computational model (116). This code was employed to solve Problem (118). Suitable variations of the code were considered in order to produce the simulations of that example. The parallelization of the scheme is not provided, though it is worth pointing out that the task is straightforward.

```
function [U,V]=fpde
a=0.8;
c=0.3;
d=0.1;
D1=0.01;
D2=0.6;
alpha=1.2;
beta=1.2;
T=2000;
L=100;

h=1/3;
tau=0.02;
Ru=tau*D1/h^alpha;
Rv=tau*D2/h^beta;

x=0:h:L;
M=length(x);
N=floor(T/tau);

ga=zeros(1,M);
gb=zeros(1,M);
ga(1)=gamma(alpha+1)/gamma((alpha/2)+1)^2;
gb(1)=gamma(beta+1)/gamma((beta/2)+1)^2;
for k=1:(M-1)
ga(k+1)=(1-(1+alpha)/((alpha/2)+k))*ga(k);
gb(k+1)=(1-(1+beta)/((beta/2)+k))*gb(k);
end

Ha=zeros(M);
Hb=zeros(M);

for j=1:M
for i=1:M
Ha(j,i)=ga(abs(i-j)+1);
Hb(j,i)=gb(abs(i-j)+1);
end
end

x0=(a*c-c+d)/a/c;
y0=(c-d)*x0/d;

U=zeros(M);
U(130:170,130:170)=0.2*ones(length(130:170));
V=normrnd(y0,0.01,M,M);

for i=1:N
W=a.*U.*(1-U)-U.*V./(U+V);
Z=c.*U.*V./(U+V)-d*V;
U=U+tau.*W-Ru.*Ha*U-Ru.*U*Ha;
V=V+tau.*Z-Rv.*Hb*V-Rv.*V*Hb;
end
end
```

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2. A positive and bounded convergent scheme for general space-fractional diffusion-reaction systems with inertial times

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A positive and bounded convergent scheme for general space-fractional diffusion-reaction systems with inertial times

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ABSTRACT

We consider a multidimensional system of hyperbolic equations with fractional diffusion, constant damping and nonlinear reactions. The system considers fractional Riesz derivatives, and generalizes many models from science. In particular, the system describes the dynamics of populations with temporal delays, whence the need to approximate nonnegative and bounded solutions is an important numerical task. Motivated by these facts, we propose a scheme to approximate the solutions. We prove the existence of the solutions under suitable regularity assumptions on the reaction functions. We prove that the scheme is capable of preserving positivity and boundedness. The technique has consistency of the second order in space and time. Using a discrete form of the energy method, we establish the stability and the convergence. As a corollary, we prove the uniqueness of the solutions. Some computer simulations in the two- and the three-dimensional scenarios are provided at the end of this work for illustration purposes.

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1. Introduction

The design of structure-preserving techniques to solve systems of partial differential equations is an important avenue of research in numerical analysis. In a broadest sense, *structure-preserving techniques* are numerical methods which are able to preserve distinctive features of some relevant solutions of a system of partial differential equations. For example, the relevant solutions of problems involving the growth of populations of bacteria must be nonnegative at all spatial points and at each time [4]. In those cases, solutions which may take on negative values are meaningless, and the condition of positivity is an important feature of the physically realistic solutions of those problems [76]. In other problems, the condition of the boundedness of the solutions may be an important characteristic of the solutions. Such is the case in those problems in which there exist natural limitations for a physical quantity of the problem. In particular, the preservation of the boundedness in systems of partial differential equations describing the growth of colonies of bacteria in a biological culture is a fundamental characteristic of the solutions of those models [44]. Other important features of the solutions of systems of partial differential equations may include the monotonicity [3] and the convexity of solutions [71]. However, the adjective 'structure-preserving' may be applied to any scheme which is capable of preserving an essential feature of the solutions of interest. Nowadays, this concept has been adopted by areas outside of numerical analysis of partial differential equations [1,70,74].

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It is important to point out that the family of structure-preserving techniques for partial differential equations is also called *dynamically consistent methods* [43]. Also, it is worthwhile to point out that this family includes the class of numerical methods which are able to preserve the energy or the mass of a physical system. Nowadays, the investigation of energy-conserving schemes is also an important avenue of research. Historically, this area of study was initiated by the beginning of the 1980s [2], but it started to receive a more considerable amount of attention since the publication of some seminal works by L. Vázquez and coauthors in the 1990s. Some of those articles report on energy-conserving numerical schemes to solve partial differential equations like the nonlinear Schrödinger equation from quantum mechanics [66], the sine-Gordon equation from quantum field theory [6], the nonlinear Klein–Gordon equations from relativistic quantum mechanics [64] and some conservative systems of ordinary differential equations [16]. In those manuscripts, the authors proved mathematically the energy-preservation characteristics of their schemes, in agreement with the associated continuous models. In proving those properties, they used the discrete energy method to show analytically the stability and the convergence of the schemes. After the publication of those reports, the design and analysis of energy-preserving schemes became a fruitful topic of research in numerical analysis. As examples, some energy-preserving methods have been proposed to simulate the nonlinear dynamics of three-dimensional beams undergoing finite rotations [26] and exact rods [60].

The decades that followed the publication of those seminal reports by Vázquez and coworkers have witnessed an increased interest in the development and analysis of energy-conserving for systems of partial differential equations. In particular, some articles by D. Furihata and coauthors have become a landmark in the development of energy-preserving finite-difference schemes for physical systems [19]. In particular, the authors of those works provided some solid reviews of various existing energy-based methods, which were designed to solve hyperbolic nonlinear partial differential equations that conserved or dissipated the energy [20]. Ultimately, those works led to the creation of the *discrete variational derivative method*, which nowadays is a powerful structure-preserving tool used to design discrete models that resemble the variational features of their continuous systems [21]. There are various reports in which the discrete variational derivative method has been employed successfully, including some works on the resolution of nonlinear systems of partial differential equations with variable coefficients [28], the investigation of numerical schemes using average-difference approaches [22], the two-dimensional vorticity equation [65] and the investigation of coupled partial differential equations through an alternating form of the discrete variational derivative method [33], among other interesting works. This approach has been extended to consider different discretization methods, including finite elements [27], finite volumes and Galerkin techniques [42], among other types of approaches [67,68].

In this work, we will investigate a general mathematical model consisting of hyperbolic partial differential equations that include the presence of nonlinear reaction terms. The system is sufficiently broad to describe many mathematical models in biology, physics and chemistry. In particular, the model may be employed to describe the space-time interactions of different populations, like diffusive predator-prey systems with an Allee effect in the prey and temporal delays [57]. As a consequence, it is indispensable to be able to guarantee the preservation of the positivity of the solutions. Motivated by these facts, we will propose a positivity- and boundedness-preserving finite-difference scheme to approximate the solutions of our system. The numerical model will be a nonlinear technique, and we will establish the existence of solutions using Brouwer's fixed-point theorem. Moreover, the capability of our scheme to preserve the positive and bounded character of the solutions will be established rigorously after imposing adequate conditions on the discretized reaction terms. In summary, a structure-preserving method will be proposed to solve our continuous problem [14,41].

To make our approach even more general, the mathematical system considered in this work will include fractional diffusion of the Riesz type [29,49]. In recent years, fractional differential equations have been used in physical models to obtain more precise descriptions of real-life phenomena [15,18,30,31,40,63,72]. As a consequence, various authors have applied fractional calculus to problems in a wide range of scientific areas [38,39], including some phenomena of viscoelasticity [32], problems associated to thermoelasticity [56], the modelling in mathematical finance [61], dynamical systems consisting of self-similar proteins [24], quantum field theory [46], the control of diabetes [62], the theory of solitary waves [77] and the physics of plasma [23]. Moreover, the investigation of population systems and, in particular, the modelling of the interactions between populations of predators and preys, has also seen a substantial progress derived from the use of fractional calculus. Indeed, some recent works have investigated fractional predator-prey systems which incorporate feedback control and a constant prey refuge [35], bifurcations of delayed fractional systems with incommensurate orders [25], periodic solutions and control optimization of models with two types of harvesting [75], fractional predator-prey systems with delay and Holling type-II functional response [59], among other recent works available in the literature. It is well known that fractional systems are computationally mode difficult to solve than classical integer-order models. In that sense, the search for computationally efficient algorithms to simulate fractional systems is still open problem of investigation.

This manuscript is organized as follows. Section 2 will present the continuous model under investigation, together with helpful analytic assumptions on the reaction terms and the crucial concepts to provide a consistent discretizations of the space-fractional derivatives, namely, the fractional-order centred differences. Some important properties of these differences will be recalled from the literature, for the sake of convenience. Section 3 will be devoted to introduce the discrete nomenclature and the discrete model to solve our continuous hyperbolic system. In that section we will establish the most important structural properties of our method. More precisely, we will show that the scheme proposed in this work is solvable, and that it conditionally positive and bounded. In turn, Section 4 will present the most relevant numerical properties of the discrete model. Concretely, we will show that the model is quadratically consistent, stable and convergent. As a consequence of stability, we will establish the uniqueness of the numerical solutions. Some numerical simulations will be presented for illustration purposes, and we will close this work with a section of conclusions.

2. Preliminaries

Throughout, let $I_s = \{1, 2, \dots, s\}$ and $\bar{I}_s = I_s \cup \{0\}$, for each $s \in \mathbb{N}$. Let $p \in \mathbb{N}$ represent the number of dimensions, assume that $T > 0$ is a fixed time, and let $a_i, b_i \in \mathbb{R}$ satisfy $a_i < b_i$, for each $i \in I_p$. Define the spatial domain $B = (a_1, b_1) \times (a_2, b_2) \times \dots \times (a_p, b_p)$, and the space-time domain $\Omega = B \times (0, T)$. Moreover, we will use $\overline{B}$ and $\overline{\Omega}$ to represent respectively the closures of B and Ω in the standard topology of $\mathbb{R}^{p+1}$, and let ∂B denote the boundary of B. We fix $q \in \mathbb{N}$, and let $u_1, u_2, \dots, u_q : \overline{\Omega} \to \mathbb{R}$ represent sufficiently smooth functions. We also define $x = (x_1, x_2, \dots, x_p)$, for each $x \in B$.

Definition 2.1 (Podlubny [55]): Assume that $f : \mathbb{R} \to \mathbb{R}$ is a function, and suppose that $n \in \mathbb{N} \cup \{0\}$ and $\alpha \in \mathbb{R}$ are such that $n - 1 < \alpha < n$. We define the *Riesz fractional derivative* of f of order α at $x \in \mathbb{R}$ (when it exists) as

$$\frac{d^\alpha f(x)}{d|x|^\alpha} = \frac{-1}{2\cos(\frac{\pi\alpha}{2})\Gamma(n-\alpha)} \frac{\mathrm{d}^n}{\mathrm{d}x^n} \int_{-\infty}^{\infty} \frac{f(\xi)\,\mathrm{d}\xi}{|x-\xi|^{\alpha+1-n}}. \tag{1}$$

Definition 2.2: Let $u : \overline{\Omega} \to \mathbb{R}$ and $i \in I_p$. Let $\alpha > -1$, and assume that n is a nonnegative integer such that $n - 1 < \alpha \leq n$. If it exists, the *Riesz space-fractional derivative* of u of order α with respect to x_i at the point $(x, t) \in \Omega$ is defined by

$$\frac{\partial^\alpha u(x,t)}{\partial |x_i|^\alpha} = \frac{-1}{2\cos(\frac{\pi\alpha}{2})\Gamma(n-\alpha)} \frac{\partial^n}{\partial x_i^n} \int_{a_i}^{b_i} \frac{u(x_1, \dots, x_{i-1}, \xi, x_{i+1}, \dots, x_p, t)\,\mathrm{d}\xi}{|x_i - \xi|^{\alpha+1-n}}. \tag{2}$$

In case that all these Riesz space-fractional derivatives of u exist at the point $(x,t) \in \Omega$, then we define the *Riesz space-fractional Laplacian* of u of order α at (x,t) by

$$\Delta^\alpha u(x,t) = \sum_{i=1}^{p} \frac{\partial^\alpha u(x,t)}{\partial |x_i|^\alpha}. \tag{3}$$

For the remainder, we let $\lambda_j, d_j \in \mathbb{N}$ and $\gamma_j \geq 0$, for each $j \in I_q$. Also, we agree that $\alpha_j \in \mathbb{R}$ is such that $1 < \alpha_j \leq 2$, for each $j \in I_q$. Meanwhile, the functions $\phi_{u_j}, \psi_{u_j} : \overline{B} \to \mathbb{R}$ will be sufficiently smooth, and we will suppose that $f_j : \mathbb{R}^q \to \mathbb{R}$ is continuously differentiable, for each $j \in I_q$. The model under investigation is described by the following initial-boundary problem, for each $(x,t) \in \Omega$:

$$\begin{aligned}
\lambda_1 \frac{\partial^2 u_1(x,t)}{\partial t^2} + \gamma_1 \frac{\partial u_1(x,t)}{\partial t} &= d_1 \Delta^{\alpha_1} u_1(x,t) + f_1(u_1(x,t), u_2(x,t), \ldots, u_q(x,t)),\\
\lambda_2 \frac{\partial^2 u_2(x,t)}{\partial t^2} + \gamma_2 \frac{\partial u_2(x,t)}{\partial t} &= d_2 \Delta^{\alpha_2} u_2(x,t) + f_2(u_1(x,t), u_2(x,t), \ldots, u_q(x,t)),\\
&\vdots\\
\lambda_q \frac{\partial^2 u_q(x,t)}{\partial t^2} + \gamma_q \frac{\partial u_q(x,t)}{\partial t} &= d_q \Delta^{\alpha_q} u_q(x,t) + f_q(u_1(x,t), u_2(x,t), \ldots, u_q(x,t)),\\
\text{such that } &\begin{cases} u_j(x,0) = \phi_{u_j}(x), & \forall j \in I_q,\ \forall x \in B,\\ \dfrac{\partial u_j(x,0)}{\partial t} = \psi_{u_j}(x) & \forall j \in I_q,\ \forall x \in B,\\ u_j(x,t) = 0, & \forall j \in I_q,\ \forall (x,t) \in \partial B \times [0,T]. \end{cases}
\end{aligned} \tag{4}$$

It is obvious that the model (4) is a fractional generalization of various systems appearing in mathematical biology, physics and chemistry. For example, that system extends to the fractional and hyperbolic scenarios various predator-prey models under different biological and analytical assumptions [7,54]. Also, this model extends the well-known sine-Gordon, the double sine-Gordon and the Klein–Gordon equations from relativistic quantum mechanics [36,64]. Moreover, (4) also generalizes some well-known models from mathematical chemistry which describe the interaction between an activator substance and an inhibitor [12,13,45]. It is important to point out that some of the models mentioned above are systems which exhibit the presence of complex patterns, and that their analysis is also an interesting topic of research from both the practical and the theoretical points of view.

In addition to describing various problems in science and engineering, the system (4) may also serve as a model for physical problems which consider energy-like physical quantities. Such is the situation for the Klein–Gordon forms of our mathematical model. In those scenarios, it is important to consider local energy densities and total energy functionals associated to (4). In our case, we will require those conditions to use a discrete form of the energy method, and establish the stability and the convergence of the scheme proposed in this work. To that end, we will suppose that there exist smooth functions $G_j : \mathbb{R}^q \to \mathbb{R}$ for each $j \in I_q$, such that the following is satisfied:

$$f_j = \frac{\partial G_j}{\partial u_j}, \quad \forall j \in I_q. \tag{5}$$

Throughout, we will let $G = (G_1, G_2, \ldots, G_q)$. In light of the additional condition (5), we can rewrite (4) as

$$\begin{aligned}
\lambda_1 \frac{\partial^2 u_1(x,t)}{\partial t^2} + \gamma_1 \frac{\partial u_1(x,t)}{\partial t} &= d_1 \Delta^{\alpha_1} u_1(x,t) + \frac{\partial G_1}{\partial u_1}(u_1(x,t), u_2(x,t), \ldots, u_q(x,t)),\\
\lambda_2 \frac{\partial^2 u_2(x,t)}{\partial t^2} + \gamma_2 \frac{\partial u_2(x,t)}{\partial t} &= d_2 \Delta^{\alpha_2} u_2(x,t) + \frac{\partial G_2}{\partial u_2}(u_1(x,t), u_2(x,t), \ldots, u_q(x,t)),
\end{aligned}$$

$$\vdots$$

$$\lambda_q \frac{\partial^2 u_q(x,t)}{\partial t^2} + \gamma_q \frac{\partial u_q(x,t)}{\partial t} = d_q \Delta^{\alpha_q} u_q(x,t) + \frac{\partial G_q}{\partial u_q}(u_1(x,t), u_2(x,t), \ldots, u_q(x,t)),$$

$$\text{such that } \begin{cases} u_j(x,0) = \phi_{u_j}(x), & \forall j \in I_q,\ \forall x \in B, \\ \dfrac{\partial u_j(x,0)}{\partial t} = \psi_{u_j}(x) & \forall j \in I_q,\ \forall x \in B, \\ u_j(x,t) = 0, & \forall j \in I_q,\ \forall (x,t) \in \partial B \times [0,T]. \end{cases} \tag{6}$$

Definition 2.3: We $L_1^x(\overline{\Omega})$ and $L_2^x(\overline{\Omega})$ be the sets of functions $f : \overline{\Omega} \to \mathbb{R}$ such that $f(\cdot,t) \in L_1(\overline{B})$ and $f(\cdot,t) \in L_2(\overline{B})$, respectively, for all $t \in [0,T]$. For each $f, g \in L_2^x(\overline{\Omega})$, the inner product of f and g is the function of t defined as

$$\langle f, g \rangle = \int_B f(\xi,t) g(\xi,t) \, d\xi, \quad \forall t \in [0,T]. \tag{7}$$

In turn, we define the norm of the function $f \in L_2^x(\overline{\Omega})$ as $\|f\|_2 = \sqrt{\langle f, f \rangle}$, for each $t \in [0,T]$. Further, the norm of the function $f \in L_1^x(\overline{\Omega})$ will be the function of t given by the identity

$$\|f\|_1 = \int_B |f(\xi,t)| \, d\xi, \quad \forall t \in [0,T]. \tag{8}$$

Let $\mathcal{V}$ be a vector space over the field $F = \mathbb{R}, \mathbb{C}$, suppose that $\langle \cdot, \cdot \rangle_{\mathcal{V}} : \mathcal{V} \times \mathcal{V} \to F$ is an inner product on $\mathcal{V}$, and assume that $T : \mathcal{V} \to \mathcal{V}$ is a linear operator. Recall that T is *self-adjoint* if $\langle Tx, y \rangle_{\mathcal{V}} = \langle x, Ty \rangle_{\mathcal{V}}$, for each $x, y \in \mathcal{V}$. Meanwhile, we say that T is *positive* if $\langle Tx, x \rangle_{\mathcal{V}} \geq 0$, for each $x \in \mathcal{V}$. An important result from functional analysis establishes that every positive self-adjoint operator over a Hilbert space has a unique positive square-root operator [17]. Moreover, the Riesz fractional derivative of order α with respect to x_i is a negative self-adjoint operator [34], for each $i \in I_p$. As a consequence, the additive inverse of the Riesz fractional derivative of order α with respect to x_i has a unique positive square-root operator, and it has the following property, for any functions $u, v : \overline{\Omega} \to \mathbb{R}$:

$$\left\langle -\frac{\partial^\alpha u}{\partial |x_i|^\alpha}, v \right\rangle = \left\langle \frac{\partial^{\alpha/2} u}{\partial |x_i|^{\alpha/2}}, \frac{\partial^{\alpha/2} v}{\partial |x_i|^{\alpha/2}} \right\rangle = \left\langle u, -\frac{\partial^\alpha v}{\partial |x_i|^\alpha} \right\rangle, \quad \forall i \in I_p,\ \forall t \in [0,T]. \tag{9}$$

Definition 2.4: Let $u : \overline{\Omega} \to \mathbb{R}$ and suppose that $\alpha \in (1,2]$. We define the fractional gradient operator of u of order $\alpha/2$ as the vector function on $\mathbb{R}^p$ given by

$$\nabla^{\alpha/2} u(x,t) = \left(\frac{\partial^{\alpha/2} u(x,t)}{\partial |x_1|^{\alpha/2}}, \frac{\partial^{\alpha/2} u(x,t)}{\partial |x_2|^{\alpha/2}}, \ldots, \frac{\partial^{\alpha/2} u(x,t)}{\partial |x_p|^{\alpha/2}} \right), \quad \forall (x,t) \in \Omega. \tag{10}$$

For the remainder, we will agree that $u = (u_1, u_2, \ldots, u_q)$. Additionally, we use the next definition from the literature [47,48,50–52]. That definition is an essential tool to provide the approximation of the Riesz space-fractional derivative of a function, and it gives us a consistent discretization of the problem (4).

Definition 2.5 (Ortigueira [48]): Let $f : \mathbb{R} \to \mathbb{R}$ be any function, and assume that $h > 0$ and $\alpha > -1$. The *fractional-order centred difference* of order α of f at the point x is defined (when it exists) as

$$\Delta_h^{(\alpha)} f(x) = \sum_{k=-\infty}^{\infty} g_k^{(\alpha)} f(x - kh), \quad \forall x \in \mathbb{R}, \tag{11}$$

where

$$g_k^{(\alpha)} = \frac{(-1)^k \Gamma(\alpha + 1)}{\Gamma(\frac{\alpha}{2} - k + 1)\Gamma(\frac{\alpha}{2} + k + 1)}, \quad \forall k \in \mathbb{Z}. \tag{12}$$

Lemma 2.6 (Wang *et al.* [73]): *Let* $0 < \alpha \leq 2$ *and* $\alpha \neq 1$.

(a) *The coefficients* $(g_k^{(\alpha)})_{k=-\infty}^{\infty}$ *satisfy*

$$g_0^{(\alpha)} = \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha/2 + 1)^2}, \quad g_{k+1}^{(\alpha)} = \left(1 - \frac{\alpha + 1}{\alpha/2 + k + 1}\right) g_k, \quad \forall k \in \mathbb{N} \cup \{0\}. \tag{13}$$

(b) $g_0^{(\alpha)} > 0$.

(c) $g_k^{(\alpha)} = g_{-k}^{(\alpha)} < 0$ *for all* $k \neq 0$.

(d) $\sum_{k=-\infty}^{\infty} g_k^{(\alpha)} = 0$. *This implies that* $g_0^{(\alpha)} = -\sum_{\substack{k=-\infty \\ k \neq 0}}^{\infty} g_k^{(\alpha)}$.

Lemma 2.7 (Wang *et al.* [73]): *Let* $f \in \mathcal{C}^5(\mathbb{R})$, *and assume that all its derivatives up to order five are integrable. If* $0 < \alpha \leq 2$ *and* $\alpha \neq 1$ *then, for almost all* $x \in \mathbb{R}$,

$$-\frac{\Delta_h^{\alpha} f(x)}{h^{\alpha}} = \frac{\partial^{\alpha} f(x)}{\partial |x|^{\alpha}} + \mathcal{O}(h^2). \tag{14}$$

Precisely, property (14) *is satisfied in all* $\mathbb{R}$ *except in a set of zero Lebesgue measure.*

3. Numerical model

We propose now a model based on finite-differences to approximate the solutions of (4). To that end, we will use the concept of fractional centred differences to approximate the spatial Riesz fractional derivatives of (4). For the remainder, we let $M_1, M_2, \ldots, M_p \in \mathbb{N}$, and fix uniform partitions of $[a_i, b_i]$, for each $i \in I_p$, by setting

$$\begin{aligned}
a_1 &= x_{1,0} < x_{1,1} < \ldots < x_{1,l_1} < \ldots < x_{1,M_1} = b_1, \quad \forall l_1 \in \bar{I}_{M_1}, \\
a_2 &= x_{2,0} < x_{2,1} < \ldots < x_{2,l_2} < \ldots < x_{2,M_2} = b_2, \quad \forall l_2 \in \bar{I}_{M_2}, \\
&\vdots \\
a_p &= x_{p,0} < x_{p,1} < \ldots < x_{p,l_p} < \ldots < x_{p,M_p} = b_p, \quad \forall l_p \in \bar{I}_{M_p},
\end{aligned} \tag{15}$$

It is obvious that $x_{i,l_i} = a_i + h_{x_i} l_i$, for each $i \in I_p$ and $l_i \in \bar{I}_{M_i}$. Here, $h_{x_i} = (b_i - a_i)/M_i$ is the partition norm in the x_i direction, for each $i \in I_p$. Analogously, we will let $K \in \mathbb{N}$ and fix a uniform partition of the temporal interval $[0, T]$ with norm equal to $\tau = T/K$, whose nodes will be represented by

$$0 = t_0 < t_1 < \ldots < t_k < \ldots < t_K = T, \quad \forall k \in \bar{I}_K. \tag{16}$$

Let $J = I_{M_1-1} \times I_{M_2-1} \times \cdots \times I_{M_p-1}$ and $\bar{J} = \bar{I}_{M_1} \times \bar{I}_{M_2} \times \cdots \times \bar{I}_{M_p}$. Define $u_{j,l}^k = u_j(x_l, t_k)$, where $x_l = (x_{1,l_1}, x_{2,l_2}, \ldots, x_{p,l_p})$, for each $j \in I_q$, $l = (l_1, l_2, \ldots, l_p) \in \bar{J}$ and $k \in \bar{I}_K$. Let

$$h = (h_{x_1}, h_{x_2}, \ldots, h_{x_p}) \in \mathbb{R}^p, \tag{17}$$

$$h_* = h_{x_1} h_{x_2} \cdots h_{x_p}. \tag{18}$$

For convenience, we define the grid $\mathcal{R}_h = \{x_l \in \bar{B} : l \in \bar{J}\}$. Moreover, we use the symbol $\mathcal{V}_h$ to denote the set of all real-valued functions define on $\bar{B}$, which vanish on all points $x \in \mathcal{R}_h \cap \partial B$. In general, if $V \in \mathcal{V}_h$ then we will set $V_l = V(x_l)$, for each $l \in \bar{J}$. In particular, we will employ the nomenclature $U_{j,l}^k$ to denote a numerical approximation to the exact value of $u_{j,l}^k$, for each $j \in I_q$ and $(l,k) \in \bar{J} \times \bar{I}_K$. Under these circumstances, it is obvious that $(U_{j,l}^k)_{l \in \bar{J}}$ is a member of $\mathcal{V}_h$, which will be represented by U_j^k for the sake of simplicity. Moreover, we will convey that $U^k = (U_1^k, U_2^k, \ldots, U_q^k)$, for each $k \in \bar{I}_K$, and we will set $U = (U^k)_{k \in \bar{I}_K}$ for the sake of simplicity.

Definition 3.1: Let $v : \bar{\Omega} \to \mathbb{R}$ be any function, and let $\alpha \in (0,1) \cup (1,2]$. Throughout this work, we will let $v_l^k = v(x_l, t_k)$, for each $(l,k) \in \bar{J} \times \bar{I}_K$. Using this nomenclature, we define the discrete average $\mu_t v_l^k = \frac{1}{2}(v_l^{k+1} + v_l^k)$, for each $(l,k) \in \bar{J} \times \bar{I}_{K-1}$. Moreover, we introduce the discrete linear difference operators

$$\delta_t v_l^k = \frac{v_l^{k+1} - v_l^k}{\tau}, \quad \forall (l,k) \in \bar{J} \times \bar{I}_{K-1}, \tag{19}$$

$$\delta_t^{(1)} v_l^k = \frac{v_l^{k+1} - v_l^{k-1}}{2\tau}, \quad \forall (l,k) \in \bar{J} \times I_{K-1}, \tag{20}$$

$$\delta_t^{(2)} v_l^k = \frac{v_l^{k+1} - 2v_l^k + v_l^{k-1}}{\tau^2}, \quad \forall (l,k) \in \bar{J} \times I_{K-1}, \tag{21}$$

$$\delta_{x_i}^{(\alpha)} v_l^k = -\frac{1}{h_{x_i}^\alpha} \sum_{n=0}^{M_i} g_{l_i-n}^{(\alpha)} v_{l_1,\ldots,l_{i-1},n,l_{i+1},\ldots,l_p}^k, \quad \forall i \in I_p,\ \forall (l,k) \in J \times \bar{I}_K \tag{22}$$

and

$$\Delta_x^{(\alpha)} v_l^k = \sum_{i=1}^{p} \delta_{x_i}^{(\alpha)} v_l^k. \tag{23}$$

Also, define $\nabla_x^{(\alpha)} v_l^k = (\delta_{x_1}^{(\alpha)} v_l^k, \delta_{x_2}^{(\alpha)} v_l^k, \ldots, \delta_{x_p}^{(\alpha)} v_l^k)$, for each $(l,k) \in \bar{J} \times \bar{I}_K$. Suppose now that $G_j : \mathbb{R}^q \to \mathbb{R}$ is differentiable in its jth component, for each $j \in I_q$, and let $u = (u_1, u_2, \ldots, u_q)$, where $u_j : \bar{\Omega} \to \mathbb{R}$ is any function, for each $j \in I_q$. If $j \in I$ and $(l,k) \in J \times I_{K-1}$ then we also define the nonlinear discrete operators

$$\begin{aligned} \delta_{u_j} G(u_l^k) = (u_{j,l}^{k+1} - u_{j,l}^{k-1})^{-1} [&G_j(u_{1,l}^k, \ldots, u_{j-1,l}^k, u_{j,l}^{k+1}, u_{j+1,l}^k, \ldots, u_{q,l}^k) \\ &- G_j(u_{1,l}^k, \ldots, u_{j-1,l}^k, u_{j,l}^{k-1}, u_{j+1,l}^k, \ldots, u_{q,l}^k)], \end{aligned} \tag{24}$$

if $u_{j,l}^{k+1} \neq u_{j,l}^{k-1}$, and by

$$\delta_{u_j} G(u_l^k) = \frac{\partial G_j(u_{1,l}^k, u_{2,l}^k, \ldots, u_{q,l}^k)}{\partial u_j}, \tag{25}$$

otherwise.

It is well known that (19) provides a first-order consistent approximation to the partial derivative of v with respect to t at (x_l, t_k). Also, the operators (20) and (21) provide second-order approximations to the first- and second-order partial derivatives of v with respect t, respectively, at the point (x_l, t_k). By Lemma 2.7, the operators (22) provide second-order approximations to the Riesz space-fractional derivative of the function v with respect to x_i at the point (x_l, t_k). In turn, this fact implies that the operator (23) yields second-order estimates of the fractional Laplacian of v. Finally, the nonlinear operators introduced in Definition 3.1 provide second-order approximations to the first derivative of the function G_j with respect u_j, for each $j \in I_q$. These facts will be used extensively in establishing the consistency property of the finite-difference scheme featured in this manuscript.

In what follows, we will let ∂J be the set of indexes $l \in \bar{J}$, such that $x_l \in \partial B$. With this notation at hand, the finite-difference method to approximate the solutions of (6) is provided by the nonlinear system of difference equations

$$\begin{array}{l}
\lambda_1 \delta_t^{(2)} U_{1,l}^k + \gamma_1 \delta_t^{(1)} U_{1,l}^k = d_1 \Delta_x^{(\alpha_1)} U_{1,l}^k + \delta_{u_1} G(U_l^k), \quad \forall (l,k) \in J \times \bar{I}_{K-1}, \\
\lambda_2 \delta_t^{(2)} U_{2,l}^k + \gamma_2 \delta_t^{(1)} U_{2,l}^k = d_2 \Delta_x^{(\alpha_2)} U_{2,l}^k + \delta_{u_2} G(U_l^k), \quad \forall (l,k) \in J \times \bar{I}_{K-1}, \\
\qquad\qquad \vdots \\
\lambda_q \delta_t^{(2)} U_{q,l}^k + \gamma_q \delta_t^{(1)} U_{q,l}^k = d_q \Delta_x^{(\alpha_q)} U_{q,l}^k + \delta_{u_q} G(U_l^k), \quad \forall (l,k) \in J \times \bar{I}_{K-1}, \\
\text{such that } \left\{ \begin{array}{ll}
U_{j,l}^0 = \phi_{u_j}(x_l), & \forall j \in I_q, \ \forall l \in J, \\
\delta_t^{(1)} U_{j,l}^0 = \psi_{u_j}(x_l), & \forall j \in I_q, \ \forall l \in J, \\
U_{j,l}^k = 0, & \forall j \in I_q, \ \forall (l,k) \in \partial J \times \bar{I}_K.
\end{array} \right.
\end{array} \tag{26}$$

Obviously, the system (26) is a three-step scheme. Moreover, the fact that the function G may be in general nonlinear makes this discrete model a nonlinear technique to approximate the solutions of (6). We will prove that this scheme satisfies various structural and numerical properties. To that end, we will require some additional conventions, and we will need to recall some more results from the literature.

Definition 3.2: We introduce, respectively, the inner product $\langle \cdot, \cdot \rangle : \mathcal{V}_h \times \mathcal{V}_h \to \mathbb{R}$ and the norm $\| \cdot \|_1 : \mathcal{V}_h \to \mathbb{R}$ by

$$\langle V, W \rangle = h_* \sum_{l \in J} V_l W_l, \quad \|V\|_1 = h_* \sum_{l \in J} |V_l|, \tag{27}$$

for each $V, W \in \mathcal{V}_h$. The Euclidean norm induced by $\langle \cdot, \cdot \rangle$ will be denoted by $\| \cdot \|_2$. Finally, the infinity norm on $\mathcal{V}_h$ is the function $\| \cdot \|_\infty : \mathcal{V}_h \to \mathbb{R}$ given by

$$\|V\|_\infty = \max\{|V_l| \in \mathbb{R} : l \in J\}, \quad \forall V \in \mathcal{V}_h. \tag{28}$$

Lemma 3.3 (Macías-Díaz [37]): *Let $\alpha \in (1,2]$ and $i \in I_p$, and define the constants*

$$g_h^{(\alpha)} = 2 g_0^{(\alpha)} h_* \sqrt{\sum_{i=1}^p h_{x_i}^{-2\alpha}}, \quad \mathbf{g}_h^{(\alpha)} = 2 g_0^{(\alpha)} h_* \sum_{i=1}^p h_{x_i}^{-\alpha}. \tag{29}$$

Then the following are satisfied:

(a) $\langle -\delta_{x_i}^{(\alpha)} V, W\rangle = \langle \delta_{x_i}^{(\alpha/2)} V, \delta_{x_i}^{(\alpha/2)} W\rangle = \langle V, -\delta_{x_i}^{(\alpha)} W\rangle$, *for each* $V, W \in \mathcal{V}_h$,
(b) $\|\delta_{x_i}^{(\alpha/2)} V\|_2^2 \leq 2g_0^{(\alpha)} h_* h_i^{-\alpha} \|V\|_2^2$, *for each* $V \in \mathcal{V}_h$,
(c) $\|\delta_{x_i}^{(\alpha)} V\|_2^2 = \|\delta_{x_i}^{(\alpha/2)} \delta_{x_i}^{(\alpha/2)} V\|_2^2$, *for each* $V \in \mathcal{V}_h$,
(d) $\|\delta_{x_i}^{(\alpha)} V\|_2^2 \leq 4(g_0^{(\alpha)} h_* h_i^{-\alpha})^2 \|V\|_2^2$, *for each* $V \in \mathcal{V}_h$, *and*
(e) $\sum_{i\in\mathcal{I}_p} \|\delta_{x_i}^{(\alpha)} V\|_2^2 \leq (g_h^{(\alpha)} \|V\|_2)^2$ *and* $\sum_{i\in\mathcal{I}_p} \|\delta_{x_i}^{(\alpha/2)} V\|_2^2 \leq \mathbf{g}_h^{(\alpha)} \|V\|_2^2$, *for each* $V \in \mathcal{V}_h$.

Lemma 3.4 (Brouwer's fixed-point theorem): *Let $\mathcal{V}$ be a finite-dimensional vector space over $\mathbb{R}$, and let $\langle\cdot,\cdot\rangle$ be an inner product on $\mathcal{V}$. Suppose that $F : \mathcal{V} \to \mathcal{V}$ is continuous, and that there exists $\lambda \geq 0$ such that $\langle F(w), w\rangle \geq 0$, for each $w \in \mathcal{V}$ with $\|w\| = \lambda$. Then there exists $w \in \mathcal{V}$ with $\|w\| \leq \lambda$, satisfying $F(w) = 0$.*

Theorem 3.5 (Solvability): *Let G be a smooth function with the property that the partial derivative of G_j with respect to u_j is essentially bounded, for each $j \in I_q$. Then the system* (26) *is solvable for any set of initial conditions.*

Proof: Observe that U^0 is defined explicitly through the initial conditions. Suppose now that U^{k-1} and U^k have been obtained, for some $k \in I_{K-1}$. For each $j \in I_q$, we let $F_j : \mathcal{V}_h \to \mathcal{V}_h$ the function whose lth component is denoted by $F_{j,l} : \mathcal{V}_h \to \mathbb{R}$. More precisely, for each $j \in I_q$, $l \in \bar{J}$ and $W_j \in \mathcal{V}_h$, we define

$$F_{j,l}(W_j) = \begin{cases} \frac{\lambda_j}{\tau^2}\left(W_{j,l} - 2U_{j,l}^k + U_{j,l}^{k-1}\right) + \frac{\gamma_j}{2\tau}\left(W_{j,l} - U_{j,l}^{k-1}\right) & \\ \quad -d_j \Delta_x^{(\alpha_j)} U_{j,l}^k - \delta_{w_j,u_j} G_l^k, & \text{if } l \in J, \\ 0, & \text{if } l \in \partial J. \end{cases} \tag{30}$$

Here, we agree that

$$\delta_{w_j,u_j} G_l = \begin{cases} (W_{j,l} - U_{j,l}^{k-1})^{-1}[G_j(U_{1,l}^k, \ldots, U_{j-1,l}^k, W_{j,l}, U_{j+1,l}^k, \ldots, U_{q,l}^k) & \\ \quad -G_j(U_{1,l}^k, \ldots, U_{j-1,l}^k, U_{j,l}^{k-1}, U_{j+1,l}^k, \ldots, U_{q,l}^k)], & \text{if } W_{j,l} \neq U_{j,l}^{k-1}, \\ \dfrac{\partial G(U_{1,l}^k, U_{2,l}^k, \ldots, U_{q,l}^k)}{\partial U_j}, & \text{otherwise.} \end{cases} \tag{31}$$

It is obvious that $F_{j,l}$ is continuous, for each $j \in I_q$ and $l \in \bar{J}$. Notice that the hypothesis on the regularity of G assures that there exists a constant $K_1 \geq 0$ with the property that $\|\delta_{w_j,u_j} G_l\|_2 \leq K_1$, for each $j \in I_q$, $W_j \in \mathcal{V}_h$ and $l \in \bar{J}$. On the other hand, we let $F = F_1 \times F_2 \times \ldots \times F_q : \mathcal{V}_h^q \to \mathcal{V}_h^q$ be the function given by

$$F(W_1, \ldots, W_q) = (F_1(W_1), \ldots, F_q(W_q)), \quad \forall W_1, \ldots, W_q \in \mathcal{V}_h. \tag{32}$$

Let now $W = (W_1, W_2, \ldots, W_q) \in \mathcal{V}_h^q$, take the inner product of $F(W)$ with W, use the Cauchy–Schwarz inequality and the properties of Lemma 3.3 to check that there exists a constant $K_2 \geq 0$, such that

$$\begin{aligned}\langle F(W), W\rangle = \sum_{j=1}^q \langle F_j(W_j), W_j\rangle \geq \sum_{j=1}^q \Bigg\{ &\frac{\lambda_j}{\tau}\left[\|W_j\|_2^2 - 2\|U_j^k\|_2\|W_j\|_2 - \|U_j^{k-1}\|_2\|W_j\|_2\right] \\ &+ \frac{\gamma_j}{2\tau}\left[\|W_j\|_2^2 - \|U_j^{k-1}\|_2\|W_j\|_2\right] - d_j \sum_{i=1}^p \|\delta_{x_i}^{(\alpha_j)} U_j^k\|_2\|W_j\|_2 - \|\delta_{w_j,u_j} G\|_2\|W_j\|_2 \Bigg\}\end{aligned}$$

$$
\begin{aligned}
&\geq \sum_{j=1}^{q}\left\{\frac{\lambda_j}{\tau}\|W_j\|_2\left[\|W_j\|_2-2\|U_j^k\|_2-\|U_j^{k-1}\|_2\right]+\frac{\gamma_j}{2\tau}\|W_j\|_2\left[\|W_j\|_2-\|U_j^{k-1}\|_2\right]\right.\\
&\qquad\left.-\,d_jK_2\|W_j\|_2-K_1\|W_j\|_2\right\}\\
&\quad=\sum_{j=1}^{q}\|W_j\|_2\left[c_j\|W_j\|_2-\frac{2\lambda_j}{\tau}\|U_j^k\|_2-c_j\|U_j^{k-1}\|_2-d_jK_2-K_1\right]\\
&=\sum_{j=1}^{q}c_j\|W_j\|_2\left[\|W_j\|_2-\lambda_j\right],
\end{aligned}
\tag{33}
$$

where

$$
c_j=\frac{\lambda_j}{\tau}+\frac{\gamma_j}{2\tau},\quad \forall j\in I_q, \tag{34}
$$

$$
\lambda_j=\frac{4\lambda_j\|U_j^k\|_2}{2\lambda_j+\gamma_j}+\|U_j^{k-1}\|_2+\frac{2\tau(d_jK_2+K_1)}{2\lambda_j+\gamma_j},\quad \forall j\in I_q. \tag{35}
$$

All of these constants are positive numbers, which implies that $c_* = \min\{c_j : j \in I_q\}$ is likewise positive, as are the numbers $c^* = \max\{c_j : j \in I_q\}$ and $\lambda^* = \max\{\lambda_j : j \in I_q\}$. With these conventions, it follows from (33) that

$$
\begin{aligned}
\langle F(W),W\rangle &\geq c_*\sum_{j=1}^{q}\|W_j\|_2^2-c^*\lambda^*\sum_{j=1}^{q}\|W_j\|_2\\
&\geq c_*\|W\|_2^2-c^*\lambda^*q\|W\|_2=c_*\|W\|_2(\|W\|_2-\lambda),
\end{aligned}
\tag{36}
$$

with $\lambda = c^*\lambda^*q/c_*$. Note that $\lambda > 0$, and that $\langle F(W), W\rangle \geq 0$, for each $W \in \mathbb{V}_h^q$ with $\|W\|_2 = \lambda$. Lemma 3.4 assures now that there is $U^{k+1} = (U_1^{k+1}, U_2^{k+1}, \ldots, U_q^{k+1}) \in \mathcal{V}_h^q$ with $\|U^{k+1}\|_2 \leq \lambda$, such that $F(U^{k+1}) = 0$. In particular, notice that U^{k+1} is a solution of the system (26). The case when $k = 0$ is handled similarly, except that we must consider the additional conditions provided by the discrete initial velocities. The conclusion readily follows now by induction. ■

Once we have established the existence of solutions of (26), we turn our attention to the capability of the numerical scheme to preserve the positivity and the boundedness. The conservation of these features will be of utmost importance in those problems where the variables under investigation are measured in absolute scales.

Definition 3.6: Let U be a solution of the discrete problem (26), and let $k \in \bar{I}_K$. We use the notation $U^k \geq 0$ to denote the fact that $U_{j,l}^k \geq 0$, for each $j \in I_q$ and $l \in \bar{J}$. If $\beta \in \mathbb{R}$ then we employ the nomenclature $U^k \leq \beta$ to mean that $U_{j,l}^k \leq \beta$, for each $j \in I_q$ and $l \in \bar{J}$. Finally, if $\beta > 0$ then we will use the notation $0 \leq U^k \leq \beta$ to represent that both conditions $U^k \geq 0$ and $U^k \leq \beta$ are satisfied.

Theorem 3.7 (Positivity and boundedness): *Let $\beta > 0$ and $k \in \bar{I}_{K-1}$.*

(a) *Positivity. Let $U^{k-1} \geq 0$ and $U^k \geq 0$, and suppose that $\delta_{u_j} G(V_l^k) \geq 0$ for any $j \in I_q$ and any sequence $(V^k)_{k\in\bar{I}_K}$ in $\mathcal{V}_h$. Then $U^{k+1} \geq 0$ holds whenever the following inequalities are satisfied:*

$$
2\lambda_j\leq\gamma_j\tau\quad\text{and}\quad \tau^2 d_j g_0^{(\alpha_j)}\sum_{i=1}^{p}h_{x_i}^{-\alpha_j}\leq 2\lambda_j,\quad \forall j\in I_q. \tag{37}
$$

(b) *Boundedness. Let $U^{k-1} \leq \beta$ and $0 \leq U^k \leq \beta$, and assume that $\delta_{u_j} G(V_l^k) \leq \beta$, for any $j \in I_q$ and any sequence $(V^k)_{k \in \bar{I}_K}$ in $\mathcal{V}_h$. Then $U^{k+1} \leq \beta$ if the following inequalities hold:*

$$2\lambda_j \leq \gamma_j \tau \quad \text{and} \quad \frac{2d_j \tau^2}{2\lambda_j + \gamma_j \tau} \sum_{i=1}^{p} \sum_{n=0}^{M_i} h_{x_i}^{-\alpha_j} g_{l_i-n}^{(\alpha_j)} \geq 1, \quad \forall j \in I_q. \tag{38}$$

Proof: Define the positive constants $e_j = \lambda_j/\tau^2$ and $c_j = \gamma_j/(2\tau)$, for each $j \in J$. Notice that the assumptions guarantee that $c_j - e_j > 0$, for each $j \in J$. After some algebraic manipulations and using the hypotheses of the theorem, it is easy to show that the following identities and inequalities are satisfied, for each $j \in I_q$ and $l \in J$:

$$\begin{aligned} U_{j,l}^{k+1} &= \frac{(c_j - e_j) U_{j,l}^{k-1}}{e_j + c_j} + \frac{2e_j U_{j,l}^k}{e_j + c_j} + \delta_{u_j} G(U_l^k) \\ &\quad - \frac{d_j}{e_j + c_j} \sum_{i=1}^{p} \sum_{n=0}^{M_i} h_{x_i}^{-\alpha_j} g_{l_i-n}^{(\alpha_j)} U_{j,l_1,\ldots,l_{i-1},n,l_{i+1},\ldots,l_p}^k \\ &> \frac{2e_j U_{j,l}^k}{e_j + c_j} - \frac{d_j}{e_j + c_j} \sum_{i=1}^{p} \sum_{n=0}^{M_i} h_{x_i}^{-\alpha_j} g_{l_i-n}^{(\alpha_j)} U_{j,l_1,\ldots,l_{i-1},n,l_{i+1},\ldots,l_p}^k \\ &> \frac{2e_j U_{j,l}^k}{e_j + c_j} - \frac{d_j g_0^{(\alpha_j)}}{e_j + c_j} \sum_{i=1}^{p} h_{x_i}^{-\alpha_j} U_{j,l}^k = \frac{U_{j,l}^k}{e_j + c_j} \left(2e_j - d_j g_0^{(\alpha_j)} \sum_{i=1}^{p} h_{x_i}^{-\alpha_j} \right) \\ &\geq 0. \end{aligned} \tag{39}$$

This establishes (a). To prove (b) now, we use the hypotheses, the inequality (38) and the first identity of (39) together with some algebraic simplifications. Bounding from above, we obtain that

$$\begin{aligned} U_{j,l}^{k+1} &\leq \frac{(c_j - e_j)\beta}{e_j + c_j} + \frac{2e_j \beta}{e_j + c_j} + \beta \\ &\quad - \frac{d_j}{e_j + c_j} \sum_{i=1}^{p} \sum_{\substack{n=0 \\ n \neq l_i}}^{M_i} h_{x_i}^{-\alpha_j} g_{l_i-n}^{(\alpha_j)} U_{j,l_1,\ldots,l_{i-1},n,l_{i+1},\ldots,l_p}^k \\ &\leq \beta \left(2 - \frac{d_j}{e_j + c_j} \sum_{i=1}^{p} \sum_{\substack{n=0 \\ n \neq l_i}}^{M_i} h_{x_i}^{-\alpha_j} g_{l_i-n}^{(\alpha_j)} \right) \leq \beta, \quad \forall j \in I_q, \ \forall l \in J. \end{aligned} \tag{40}$$

The conclusion of this result readily follows now. ■

Before closing this stage of our work, we would like to point out that Theorem 3.7 provides only sufficient conditions under which the positivity and the boundedness of the solutions of (4) are preserved. Obviously, one can provide weaker conditions under which these conditions are satisfied, if we impose more analytical conditions on the reaction functions. However, for purposes of this report, the conditions established in the last proposition suffice to exhibit the capability of the scheme (26) to preserve structural features of the solutions of the continuous model. In the following section, we will prove that the discrete model is also a numerically efficient technique.

4. Numerical properties

The aim of this section is to provide the main numerical properties of the finite-difference scheme (26). Concretely, we will show that the finite-difference scheme (26) has second-order consistency in both space and time, that it is stable and that it has quadratic order of convergence. In the sequel, we will employ the following continuous operators:

$$
\begin{aligned}
\mathcal{L}_1(u)) &= \lambda_1 \frac{\partial^2 u_1}{\partial t^2} + \gamma_1 \frac{\partial u_1}{\partial t} - d_1 \Delta^{\alpha_1} u_1 - \frac{\partial G}{\partial u_1}(u_1, u_2, \ldots, u_q), \quad \forall (x,t) \in \Omega, \\
\mathcal{L}_2(u) &= \lambda_2 \frac{\partial^2 u_2}{\partial t^2} + \gamma_2 \frac{\partial u_2}{\partial t} - d_2 \Delta^{\alpha_2} u_2 - \frac{\partial G}{\partial u_2}(u_1, u_2, \ldots, u_q), \quad \forall (x,t) \in \Omega, \\
&\vdots \\
\mathcal{L}_q(u) &= \lambda_q \frac{\partial^2 u_q}{\partial t^2} + \gamma_q \frac{\partial u_q}{\partial t} - d_q \Delta^{\alpha_q} u_q - \frac{\partial G}{\partial u_q}(u_1, u_2, \ldots, u_q), \quad \forall (x,t) \in \Omega.
\end{aligned} \tag{41}
$$

Using this nomenclature, we let $\mathcal{L}(u(x,t)) = (\mathcal{L}_1(u(x,t)), \mathcal{L}_2(u(x,t)), \ldots, \mathcal{L}_q(u(x,t)))$, for each $(x,t) \in \overline{\Omega}$. On the other hand, we will let $\mathbf{u}_l^k = (u_{1,l}^k, u_{2,l}^k, \ldots, u_{q,l}^k)$, for each $l \in \bar{J}$ and $k \in \bar{I}_k$. Also, we define the following operators, for each $(l,k) \in \bar{J} \times I_{K-1}$:

$$
\begin{aligned}
L_1(\mathbf{u}_l^k) &= \lambda_1 \delta_t^{(2)} u_{1,l}^k + \gamma_1 \delta_t^{(1)} u_{1,l}^k - d_1 \Delta_x^{(\alpha_1)} u_{1,l}^k - \delta_{u_1} G(u_l^k), \\
L_2(\mathbf{u}_l^k) &= \lambda_2 \delta_t^{(2)} u_{2,l}^k + \gamma_2 \delta_t^{(1)} u_{2,l}^k - d_2 \Delta_x^{(\alpha_2)} u_{2,l}^k - \delta_{u_2} G(u_l^k), \\
&\vdots \\
L_q(\mathbf{u}_l^k) &= \lambda_q \delta_t^{(2)} u_{q,l}^k + \gamma_q \delta_t^{(1)} u_{q,l}^k - d_q \Delta_x^{(\alpha_q)} u_{q,l}^k - \delta_{u_q} G(u_l^k).
\end{aligned} \tag{42}
$$

Moreover, we will set $L(\mathbf{u}_l^k) = (L_1(\mathbf{u}_l^k), L_2(\mathbf{u}_l^k), \ldots, L_q(\mathbf{u}_l^k))$, for each $(l,k) \in \bar{J} \times I_{K-1}$.

Definition 4.1: Let $u : \overline{\Omega} \to \mathbb{R}$ be any function. We define

$$
|||\mathcal{L}(\mathbf{u}) - L(\mathbf{u})|||_\infty = \max \left\{ \|\mathcal{L}(\mathbf{u}_l^k) - L(\mathbf{u}_l^k)\|_\infty : (l,k) \in \bar{J} \times I_{K-1} \right\}. \tag{43}
$$

Theorem 4.2 (Consistency): *If $u_1, u_2, \ldots, u_q \in C_{x,t}^{5,4}(\overline{\Omega})$ and G is continuously differentiable then there exist a positive constant C which is independent of τ and h, such that $|||\mathcal{L}(\mathbf{u}) - L(\mathbf{u})|||_\infty \leq C(\tau^2 + \|h\|_2^2)$.*

Proof: We will employ the usual arguments based on the use of Taylor's theorem to prove the conclusion of this theorem. To that end, let $j \in I_q$, and use the regularity of u_j and G together with Lemma 2.7 to assure that there exist nonnegative constants $C_{j,1}$, $C_{j,2}$, $C_{j,3}$ and C_{j,x_i} which are independent of τ and h, such that

$$
\left| \frac{\partial^2 u_j(x_l, k)}{\partial t^2} - \delta_t^{(2)} u_{j,l}^k \right| \leq C_{j,1} \tau^2, \tag{44}
$$

$$
\left| \frac{\partial u_j(x_l, t_k)}{\partial t} - \delta_t^{(1)} u_{j,l}^k \right| \leq C_{j,2} \tau^2, \tag{45}
$$

$$
\left| \Delta^{\alpha_j} u_j(x_l, t_k) - \Delta_x^{(\alpha_1)} u_{j,l}^k \right| \leq \sum_{i=1}^{p} C_{j,x_i} h_{x_i}^2, \tag{46}
$$

$$\left|\frac{\partial G_j}{\partial u_j}(u_{1,l}^k, u_{2,l}^k, \ldots, u_{q,l}^k) - \delta_{u_j} G(u_l^k)\right| \leq C_{j,3}\tau^2, \quad \forall j \in I_q, \tag{47}$$

for each $j \in I_q$ and $(l,k) \in \bar{J} \times I_{K-1}$. Let $C_{j,4} = \max\{C_{j,x_i} : i \in I_p\}$ and set

$$C_j = \max\{\lambda_j C_{j,1} + \gamma_j C_{j,2} + C_{j,3}, d_j C_{j,4}\}, \quad \forall j \in I_q. \tag{48}$$

Obviously, the constants C_j are independent of τ and h, for each $j \in I_q$. The conclusion follows now if we let $C = \max\{C_j : j \in I_q\}$, which is also independent of τ and h. ■

The following technical results will be required to prove the stability and convergence of our scheme.

Lemma 4.3 (Pen-Yu [53]): *Let $(\omega^n)_{n=0}^K$ and $(\rho^n)_{n=0}^K$ be finite sequences of nonnegative numbers, and suppose that there exists $C \geq 0$ such that*

$$\omega^n \leq \rho^n + C\tau \sum_{k=0}^{n-1} \omega^k, \quad \forall n \in I_K. \tag{49}$$

Then $\omega^n \leq \rho^n e^{Cn\tau}$, for each $n \in \bar{I}_K$.

Lemma 4.4: *If $(V^k)_{k\in\overline{K}}$ is a sequence in $\mathcal{V}_h$ and $\alpha \in (0,1) \cup (1,2]$ then the following hold, for all $k \in I_{K-1}$ and $i \in I_p$:*

(a) $2\langle \delta_t^{(2)} V^k, \delta_t^{(1)} V^k\rangle = \delta_t \|\delta_t V^{k-1}\|_2^2$.
(b) $4\langle -\delta_{x_i}^{(\alpha)} V^k, \delta_t^{(1)} V^k\rangle = \delta_t[2\mu_t \|\delta_{x_i}^{(\alpha/2)} V^{k-1}\|_2^2 - \tau^2 \|\delta_{x_i}^{(\alpha/2)} \delta_t V^{k-1}\|_2^2]$.

Proof: The proofs of these identities are obtained through algebraic calculations. ■

Lemma 4.5 (Macías-Díaz [37]): *Let $G \in \mathcal{C}^2(\mathbb{R}^p)$ and $G'' \in L^\infty(\mathbb{R}^p)$, and suppose that $(U^k)_{k=0}^K$, $(V^k)_{k=0}^K$ and $(R^k)_{k=0}^K$ are sequences in $\mathcal{V}_h^q$. Then there exists a nonnegative constant C_0 that depends only on G, such that*

$$2\tau \left|\sum_{k=1}^n \langle R_j^k + \widetilde{G}_j^k, \delta_t^{(1)} \varepsilon_j^k\rangle\right| \leq 2\tau \sum_{k=0}^n \|R_j^k\|_2^2 + C_0 \left(\|\varepsilon_j^0\|_2^2 + \tau \sum_{k=0}^n \|\delta_t \varepsilon_j^k\|_2^2\right), \tag{50}$$

for each $n \in I_{K-1}$ and $j \in I_q$. Here, $\varepsilon_{j,l}^k = V_{j,l}^k - U_{j,l}^k$ and $\widetilde{G}_{j,l}^k = \delta_{v_j} G(V_l^k) - \delta_{u_j} G(U_l^k)$ for each $(l,k) \in \bar{J} \times I_{K-1}$ and $j \in I_q$.

To establish the stability of the scheme (26), we will consider the problem (26) and assume that it has a solution U. Additionally, we will suppose that $\phi_{v_j}, \psi_{v_j} : \overline{B} \to \mathbb{R}$ are sufficiently smooth functions for each $j \in I_q$, and we will suppose that V is a solution of the discrete initial-boundary-value problem

$$
\begin{aligned}
&\lambda_1 \delta_t^{(2)} V_{1,l}^k + \gamma_1 \delta_t^{(1)} V_{1,l}^k = d_1 \Delta_x^{(\alpha_1)} V_{1,l}^k + \delta_{v_1} G(V_l^k), \quad \forall (l,k) \in J \times I_{K-1}, \\
&\lambda_2 \delta_t^{(2)} V_{2,l}^k + \gamma_2 \delta_t^{(1)} V_{2,l}^k = d_2 \Delta_x^{(\alpha_2)} V_{2,l}^k + \delta_{v_2} G(V_l^k), \quad \forall (l,k) \in J \times I_{K-1}, \\
&\qquad \vdots \\
&\lambda_q \delta_t^{(2)} V_{q,l}^k + \gamma_q \delta_t^{(1)} V_{q,l}^k = d_q \Delta_x^{(\alpha_q)} V_{q,l}^k + \delta_{v_q} G(V_l^k), \quad \forall (l,k) \in J \times I_{K-1}, \\
&\text{such that } \begin{cases} V_{j,l}^0 = \phi_{v_j}(x_l), & \forall j \in I_q, \ \forall l \in J, \\ \delta_t^{(1)} V_{j,l}^0 = \psi_{v_j}(x_l), & \forall j \in I_q, \ \forall l \in J, \\ V_{j,l}^k = 0, & \forall j \in I_q, \ \forall (l,k) \in \partial J \times \overline{I}_K. \end{cases}
\end{aligned} \tag{51}
$$

Moreover, in the statement of the following theorem, the constant $C_0 \geq 0$ will be as in the statement of Lemma 4.5.

Theorem 4.6 (Stability): *Suppose that the function G satisfies $G \in C^2(\mathbb{R}^p)$ and $G'' \in L^\infty(\mathbb{R}^p)$. Let U and V be the solutions of the problems* (26) *and* (51), *respectively, and let ε be as in Lemma* 4.5. *Assume also that the following inequalities are satisfied:*

$$
2C_0 \tau + \mathbf{g}_h^{(\alpha)} d_j \tau^2 < 2\lambda_j, \quad \forall j \in I_q. \tag{52}
$$

Let $\eta_j = \lambda_j - C_0 \tau - \frac{1}{2} \mathbf{g}_h^{(\alpha)} d_j \tau^2 \in \mathbb{R}$, for each $j \in I_q$, and define the nonnegative constants

$$
\rho_j = C_0 \|\varepsilon_j^0\|_2^2 + \lambda_j \|\delta_t \varepsilon_j^0\|_2^2 + d_j \sum_{i=1}^p \mu_t \|\delta_{x_i}^{(\alpha_j/2)} \varepsilon_j^0\|_2^2, \quad \forall j \in I_q, \tag{53}
$$

$$
\omega_j^n = \eta_j \|\delta_t \varepsilon_j^n\|_2^2 + d_j \sum_{i=1}^p \mu_t \|\delta_{x_i}^{(\alpha_j/2)} \varepsilon_j^n\|_2^2, \quad \forall j \in I_q, \ \forall n \in \overline{I}_{K-1}. \tag{54}
$$

There exist constants $C_j \geq 0$ which are independent of τ and h, such that $\omega_j^n \leq \rho_j e^{C_j n \tau}$, for each $j \in I_q$ and $n \in \overline{I}_K$.

Proof: Beforehand, notice that the problems (26) and (51) are solvable in light of Theorem 3.5. Notice that the sequence $(\varepsilon^k)_{k=0}^K$ satisfies the discrete initial-boundary-value problem

$$
\begin{aligned}
&\lambda_1 \delta_t^{(2)} \varepsilon_{1,l}^k + \gamma_1 \delta_t^{(1)} \varepsilon_{1,l}^k = d_1 \Delta_x^{(\alpha_1)} \varepsilon_{1,l}^k + \widetilde{G}_{1,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\lambda_2 \delta_t^{(2)} \varepsilon_{2,l}^k + \gamma_2 \delta_t^{(1)} \varepsilon_{2,l}^k = d_2 \Delta_x^{(\alpha_2)} \varepsilon_{2,l}^k + \widetilde{G}_{2,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\qquad \vdots \\
&\lambda_q \delta_t^{(2)} \varepsilon_{q,l}^k + \gamma_q \delta_t^{(1)} \varepsilon_{q,l}^k = d_q \Delta_x^{(\alpha_q)} \varepsilon_{q,l}^k + \widetilde{G}_{q,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\text{such that } \begin{cases} \varepsilon_{j,l}^0 = \phi_{v_j}(x_l) - \phi_{u_j}(x_l), & \forall j \in I_q, \ \forall l \in J, \\ \delta_t^{(1)} \varepsilon_{j,l}^0 = \psi_{v_j}(x_l) - \psi_{u_j}(x_l), & \forall j \in I_q, \ \forall l \in J, \\ \varepsilon_{j,l}^k = 0, & \forall j \in I_q, \ \forall (l,k) \in \partial J \times \overline{I}_K, \end{cases}
\end{aligned} \tag{55}
$$

where $\widetilde{G}_{j,l}^k$ is as in the statement of Lemma 4.5, for each $(l,k) \in \overline{J} \times I_{K-1}$ and $j \in I_q$. Let now $k \in I_{K-1}$ and $j \in I_q$. Take the inner product of $\delta_t^{(1)} \varepsilon_j^k$ with both sides of the jth vector equation of (55), and use then the identities of Lemma 4.4. After a straightforward substitution and rearranging terms algebraically, we obtain

$$\begin{aligned}\frac{\lambda_j}{2}\delta_t\|\delta_t\varepsilon_j^{k-1}\|_2^2 + \gamma_j\|\delta_t^{(1)}\varepsilon_j^k\|_2^2 &= \langle\widetilde{G}_j^k, \delta_t^{(1)}\varepsilon_j^k\rangle \\ &- d_j\sum_{i=1}^{p}\left[\frac{1}{2}\mu_t\|\delta_{x_i}^{(\alpha_j/2)}\varepsilon_j^{k-1}\|_2^2 - \frac{\tau^2}{4}\|\delta_{x_i}^{(\alpha_j/2)}\delta_t\varepsilon_j^{k-1}\|_2^2\right],\end{aligned} \tag{56}$$

for each $(k,j) \in I_{K-1} \times I_q$. Fix now $n \in I_{K-1}$ and take the sum on both sides of this last identity over all $k \in I_n$. Multiply then by 2τ, use the formula for telescoping sums and use Lemma 4.5 with $R^k = 0$ for all $k \in \overline{I}_K$. Rearranging terms algebraically and bounding from above, we obtain the following chain of inequalities:

$$\begin{aligned}&\left(\lambda_j - \frac{\mathbf{g}_h^{(\alpha_j)}d_j\tau^2}{2}\right)\|\delta_t\varepsilon_j^n\|_2^2 + d_j\sum_{i=1}^{p}\mu_t\|\delta_{x_i}^{(\alpha_j/2)}\varepsilon_j^n\|_2^2 \\ &\leq \lambda_j\|\delta_t\varepsilon_j^n\|_2^2 + d_j\sum_{i=1}^{p}\mu_t\|\delta_{x_i}^{(\alpha_j/2)}\varepsilon_j^n\|_2^2 - \frac{d_j\tau^2}{2}\sum_{i=1}^{p}\|\delta_{x_i}^{(\alpha_j/2)}\delta_t\varepsilon_j^n\|_2^2 \\ &\leq \lambda_j\|\delta_t\varepsilon_j^0\|_2^2 + d_j\sum_{i=1}^{p}\mu_t\|\delta_{x_i}^{(\alpha_j/2)}\varepsilon_j^0\|_2^2 + 2\tau\left|\sum_{k=1}^{n}\langle\widetilde{G}_j^k, \delta_t^{(1)}\varepsilon_j^k\rangle\right| \\ &\leq \rho_j + C_0\tau\sum_{k=0}^{n}\|\delta_t\varepsilon_j^k\|_2^2, \quad \forall j \in I_q,\ \forall n \in I_{K-1}.\end{aligned} \tag{57}$$

Let $C_j = C_0/\eta_j$, for each $j \in I_q$, and subtract $C_0\tau\|\delta_t\varepsilon_j^n\|_2^2$ from both ends of the last chain of inequalities to obtain

$$\omega_j^n \leq \rho_j + C_0\tau\sum_{k=0}^{n-1}\|\delta_t\varepsilon_j^k\|_2^2 \leq \rho_j + C_j\tau\sum_{k=0}^{n-1}\omega^k, \quad \forall j \in I_q,\ \forall n \in I_{K-1}. \tag{58}$$

The conclusion readily follows from this last inequality and Lemma 4.3. ∎

Corollary 4.7 (Uniqueness): *Let $G \in \mathcal{C}^2(\mathbb{R}^p)$ and $G'' \in L^\infty(\mathbb{R}^p)$. Assume that the inequalities* (52) *are satisfied. Then the discrete problem* (26) *has a unique solution.*

Proof: Assume that U and V are solutions of (26). Using that U and V satisfy the same initial conditions, it follows that $\varepsilon_j^0 = \delta_t\varepsilon_j^0 = \delta_{x_i}^{(\alpha_j/2)}\varepsilon_j^0 = 0$, for each $j \in I_q$ and $i \in I_p$. The conclusion of Theorem 4.6 assures that, for each $j \in I_q$ and $n \in \overline{I}_{K-1}$,

$$\begin{aligned}\frac{\eta_j}{\tau^2}\|\varepsilon_j^{n+1} - \varepsilon_j^n\|_2^2 &= \eta_j\|\delta_t\varepsilon_j^n\|_2^2 \\ &\leq \left(C_0\|\varepsilon_j^0\|_2^2 + \lambda_j\|\delta_t\varepsilon_j^0\|_2^2 + d_j\sum_{i=1}^{p}\mu_t\|\delta_{x_i}^{(\alpha_j/2)}\varepsilon_j^0\|_2^2\right)e^{C_jT} = 0.\end{aligned} \tag{59}$$

Using induction, we obtain that $\varepsilon_j^n = \varepsilon_j^0 = 0$, for each $j \in I_q$ and $n \in \overline{I}_K$. ∎

Assume now that u is the unique solution of the continuous problem (6). As a consequence, u satisfies the following discrete problem:

$$\begin{aligned}
&\lambda_1 \delta_t^{(2)} u_{1,l}^k + \gamma_1 \delta_t^{(1)} u_{1,l}^k = d_1 \Delta_x^{(\alpha_1)} u_{1,l}^k + \delta_{u_1} G(u_l^k) + R_{1,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\lambda_2 \delta_t^{(2)} u_{2,l}^k + \gamma_2 \delta_t^{(1)} u_{2,l}^k = d_2 \Delta_x^{(\alpha_2)} u_{2,l}^k + \delta_{u_2} G(u_l^k) + R_{2,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\qquad \vdots \\
&\lambda_q \delta_t^{(2)} u_{q,l}^k + \gamma_q \delta_t^{(1)} u_{q,l}^k = d_q \Delta_x^{(\alpha_q)} u_{q,l}^k + \delta_{u_q} G(u_l^k) + R_{q,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\text{such that } \begin{cases} u_{j,l}^0 = \phi_{u_j}(x_l), & \forall j \in I_q,\ \forall l \in J, \\ \delta_t^{(1)} u_{j,l}^0 = \psi_{u_j}(x_l), & \forall j \in I_q,\ \forall l \in J, \\ u_{j,l}^k = 0, & \forall j \in I_q,\ \forall (l,k) \in \partial J \times \overline{I}_K. \end{cases}
\end{aligned} \tag{60}$$

The number $R_{j,l}^k$ represents the local truncation error of the jth equation at the node (x_l, t_k), for each $j \in I_q$ and $(l,k) \in \overline{J} \times I_{K-1}$. Under the assumptions of Theorem 4.2, there is a constant $C \geq 0$ independent of τ and h, such that $|||R|||_\infty \leq C(\tau^2 + \|h\|_2^2)$. This fact will be employed implicitly in the proof of the following theorem, along with the notation and the conclusions of the previous lemmas.

Theorem 4.8 (Convergence): *Let $u \in \mathcal{C}_{x,t}^{5,4}(\overline{\Omega})$ be the unique solution of* (6), *and let $G \in \mathcal{C}^2(\mathbb{R}^p)$ and $G'' \in L^\infty(\mathbb{R}^p)$. If the inequalities* (52) *hold then the solution of the scheme* (26) *converges to u with order $\mathcal{O}(\tau^2 + \|h\|_2^2)$.*

Proof: Define the constants $\epsilon_{j,l}^k = u_{j,l}^k - U_{j,l}^k$, for each $j \in I_q$ and $(l,k) \in \overline{J} \times I_{K-1}$. It is obvious that the following discrete initial-boundary-value problem is satisfied:

$$\begin{aligned}
&\lambda_1 \delta_t^{(2)} \epsilon_{1,l}^k + \gamma_1 \delta_t^{(1)} \epsilon_{1,l}^k = d_1 \Delta_x^{(\alpha_1)} \epsilon_{1,l}^k + \widetilde{G}_{1,l}^k + R_{1,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\lambda_2 \delta_t^{(2)} \epsilon_{2,l}^k + \gamma_2 \delta_t^{(1)} \epsilon_{2,l}^k = d_2 \Delta_x^{(\alpha_2)} \epsilon_{2,l}^k + \widetilde{G}_{2,l}^k + R_{2,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\qquad \vdots \\
&\lambda_q \delta_t^{(2)} \epsilon_{q,l}^k + \gamma_q \delta_t^{(1)} \epsilon_{q,l}^k = d_q \Delta_x^{(\alpha_q)} \epsilon_{q,l}^k + \widetilde{G}_{q,l}^k + R_{q,l}^k, \quad \forall (l,k) \in J \times I_{K-1}, \\
&\text{such that } \begin{cases} \epsilon_{j,l}^0 = \phi_{v_j}(x_l) - \phi_{u_j}(x_l), & \forall j \in I_q,\ \forall l \in J, \\ \delta_t^{(1)} \epsilon_{j,l}^0 = \psi_{v_j}(x_l) - \psi_{u_j}(x_l), & \forall j \in I_q,\ \forall l \in J, \\ \epsilon_{j,l}^k = 0, & \forall j \in I_q,\ \forall (l,k) \in \partial J \times \overline{I}_K. \end{cases}
\end{aligned} \tag{61}$$

Here, we agree that $\widetilde{G}_{j,l}^k = \delta_{u_j} G(u_l^k) - \delta_{u_j} G(U_l^k)$, for each $j \in I_q$ and $(l,k) \in \overline{J} \times I_{K-1}$. We proceed now as in the proof of Theorem 4.6. More precisely, let $k \in I_{K-1}$ and $j \in I_q$. Take the inner product of $\delta_t^{(1)} \epsilon_j^k$ with both sides of the jth equation of (61), and use the identities of Lemma 4.4. After rearranging terms algebraically, we reach

$$\begin{aligned}
\frac{\lambda_j}{2} \delta_t \|\delta_t \epsilon_j^{k-1}\|_2^2 + \gamma_j \|\delta_t^{(1)} \epsilon_j^k\|_2^2 &= \langle \widetilde{G}_j^k + R_j^k, \delta_t^{(1)} \epsilon_j^k \rangle \\
&\quad - d_j \sum_{i=1}^p \left[\frac{1}{2} \mu_t \|\delta_{x_i}^{(\alpha_j/2)} \epsilon_j^{k-1}\|_2^2 - \frac{\tau^2}{4} \|\delta_{x_i}^{(\alpha_j/2)} \delta_t \epsilon_j^{k-1}\|_2^2 \right],
\end{aligned} \tag{62}$$

for each $(k,j) \in I_{K-1} \times I_q$. Let $n \in I_{K-1}$ and take the sum on both sides of this last equation over all $k \in I_n$. Multiply then by 2τ, use the formula for telescoping sums and use Lemma 4.5. Proceeding again as in the proof of Theorem 4.6 and using the case constants C_j in that proof, we may readily reach the inequalities

$$\omega_j^n \leq \rho_j^n + C_j \tau \sum_{k=0}^{n-1} \omega^k, \quad \forall j \in I_q, \, \forall n \in I_{K-1}. \tag{63}$$

Here, the constants are defined as

$$\rho_j^n = C_0 \|\epsilon_j^0\|_2^2 + \lambda_j \|\delta_t \epsilon_j^0\|_2^2 + d_j \sum_{i=1}^{p} \mu_t \|\delta_{x_i}^{(\alpha_j/2)} \epsilon_j^0\|_2^2 + 2\tau \sum_{k=0}^{n} \|R_j^k\|_2^2, \quad \forall j \in I_q, \tag{64}$$

$$\omega_j^n = \eta_j \|\delta_t \epsilon_j^n\|_2^2 + d_j \sum_{i=1}^{p} \mu_t \|\delta_{x_i}^{(\alpha_j/2)} \epsilon_j^n\|_2^2, \quad \forall j \in I_q, \, \forall n \in \bar{I}_{K-1}, \tag{65}$$

and η_j is as in the proof of Theorem 4.6, for each $j \in I_q$. Note that the initial data of the problem (61) and the conclusion of Theorem 4.2 guarantee that there exists a constant $C \geq 0$ which is independent of τ and h, with the property that $\rho_j^n \leq 2C^2 T(\tau^2 + \|h\|_2^2)^2$, for each $j \in I_q$ and $n \in \bar{I}_K$. From the inequality (63) and Lemma 4.3, we obtain

$$\eta_j \|\delta_t \epsilon_j^n\|_2^2 \leq \omega_j^n \leq \rho_j^n e^{C_j n \tau} \leq 2C^2 T(\tau^2 + \|h\|_2^2)^2 e^{C_j T}, \quad \forall j \in I_q, \, \forall n \in \bar{I}_{K-1}. \tag{66}$$

As a consequence, it follows that $\|\delta_t \epsilon_j^n\|_2 \leq K_j(\tau^2 + \|h\|_2^2)$, for each $j \in I_q$ and $n \in \bar{I}_{K-1}$ which, in turn, implies that $\|\epsilon_j^{n+1}\|_2 - \|\epsilon_j^n\|_2 \leq K_j \tau(\tau^2 + \|h\|_2^2)$. Let $k \in \bar{I}_{K-1}$ and take the sum on both sides of this inequality over all $n \in I_k$. After applying the formula for telescoping sums and using the initial data, we obtain $\|\epsilon_j^k\|_2 \leq K(\tau^2 + \|h\|_2^2)$, for each $j \in I_q$ and $k \in \bar{I}_K$. Here, we used $K = \max\{K_j T : j \in I_q\}$. The conclusion of this theorem readily follows now. ∎

5. Computer simulations

The present section will be devoted to provide simulations to illustrate the performance of the finite-difference scheme (26). Beforehand, it is important to recall that the finite-difference method is a nonlinear technique. Moreover, for each $j \in I_q$ and $(l, k) \in J \times I_{K-1}$, the corresponding difference equation of our has $u_{j,l}^k$ as the only unknown. To estimate it, one may use a standard computational technique to approximate the roots of nonlinear algebraic equations. In our case, we used a Fortran 95 implementation of the Newton–Raphson method, using a tolerance of 1×10^{-8} and a maximum number of iterations equal to 20. It is important to mention here that our computational code converged to the solution in less of 10 iterations in most of the cases. For convenience, Figure 1 provides the forward-difference stencil of the discrete model (26) when $p = q = 1$. For the sake of convenience, we used $M = M_1$ and $l = l_1$.

From a computational point of view, we need to point out that the case when $k = 0$ requires special consideration. Indeed, notice that the approximation at the fictitious time t_{-1} is required to use the finite-difference scheme. To that end, we require to employ the both initial approximations available for each $j \in I_q$, along with the jth difference equation of (26). Notice that the initial profile reads$U_{j,l}^0 = \phi_{u_j}(x_l)$, for each $j \in I_q$ and $l \in J$. Meanwhile, the discrete initial velocity yields $U_{j,l}^{-1} = U_{j,l}^1 - 2\tau \psi_{u_j}(x_l)$, for each $j \in I_q$ and $l \in J$. As a consequence of this identities and the jth difference equation of our scheme at the time $t = 0$, we obtain

$$\frac{2\lambda_j}{\tau^2} \left[U_{j,l}^1 - \phi_{u_j}(x_l) - \tau \psi_{u_j}(x_j) \right] + \gamma_j \psi_{u_j}(x_l) = d_j \Delta_x^{(\alpha_j)} \phi_{u_j}(x_l) + \frac{\Delta_{u_j} G_l^0}{2\tau \psi_{u_j}(x_l)}, \tag{67}$$

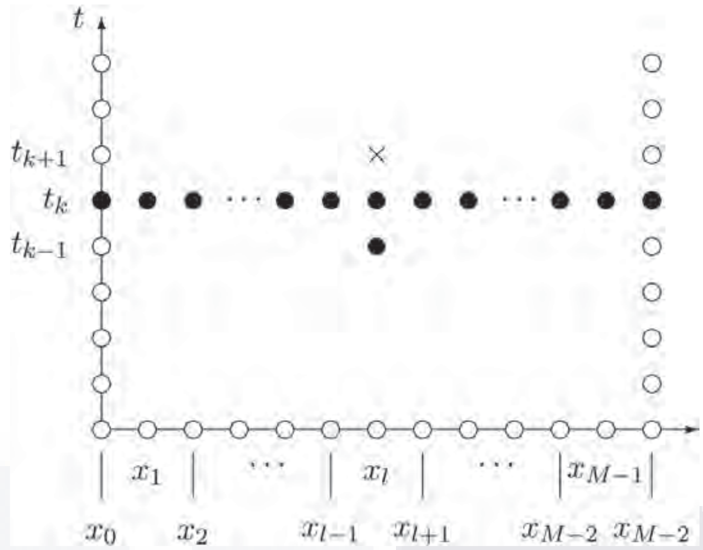

Figure 1. Forward-difference stencil for the approximation to the exact solution of (4) at the time t_k, using the finite-difference scheme (26). The black circles represent the known approximations at the times t_{k-1} and t_k, while the cross denotes the unknown approximation at the time t_{k+1}. For illustration purposes, the description refers to the case when $p = q = 1$. Moreover, we convey that $M = M_1$ and $l = l_1$.

for each $j \in J$ and $l \in J$, where

$$\begin{aligned}\Delta_{u_j} G_l^0 &= G\left(\phi_{u_1}(x_l), \ldots, \phi_{u_{j-1}}(x_l), U_{j,l}^1, \phi_{u_{j+1}}(x_l), \ldots, \phi_{u_q}(x_l)\right) \\ &\quad - G\left(\phi_{u_1}(x_l), \ldots, \phi_{u_{j-1}}(x_l), U_{j,l}^1 - 2\tau\psi_{u_j}(x_l), \phi_{u_{j+1}}(x_l), \ldots, \phi_{u_q}(x_l)\right). \end{aligned} \tag{68}$$

In this section, we will apply our numerical methodology to the investigation on the existence of Turing patterns in some hyperbolic extension of a reaction-diffusion system appearing in the investigation of some predator-prey models [5]. More concretely, we will consider the spatio-temporal version of the classical Holling–Tanner-type predator-prey system [69], and extend it to the hyperbolic and fractional scenario. That model is used in the investigation of spreading of plankton, and it illustrates the transition of Turing patterns from ‘cold’ to ‘hot’ spots through labyrinthine structures. More precisely, the model under investigation in this example is given by the system

$$\begin{aligned} &\lambda_1 \frac{\partial^2 u_1(x,t)}{\partial t^2} + \frac{\partial u_1(x,t)}{\partial t} = \Delta^{\alpha_1} u_1(x,t) + u_1(x,t)(1 - u_1(x,t)) - \frac{u_1(x,t)u_2(x,t)}{u_1(x,t) + \nu}, \\ &\lambda_2 \frac{\partial^2 u_2(x,t)}{\partial t^2} + \frac{\partial u_2(x,t)}{\partial t} = d_2 \Delta^{\alpha_2} u_2(x,t) + \theta\left(1 - \frac{\zeta u_2(x,t)}{u_1(x,t)}\right) u_2(x,t), \\ &\text{such that } \begin{cases} u_j(x,0) = \phi_{u_j}(x), & \forall j \in \{1,2\},\ \forall x \in B, \\ \dfrac{\partial u_j(x,0)}{\partial t} = \psi_{u_j}(x) & \forall j \in \{1,2\},\ \forall x \in B, \\ u_j(x,t) = 0, & \forall j \in \{1,2\},\ \forall (x,t) \in \partial B \times [0,T]. \end{cases} \end{aligned} \tag{69}$$

The model describes the space-time interaction between phytoplankton (u_1) and zooplankton (u_2) over the spatial domain $B = (0,L) \times (0,L)$. The parameters ζ, θ and ν are positive, as well as the constants λ_1, λ_2 and d_2. Here, ζ is the number of phytoplankton required to support one zooplankton at equilibrium, θ is the predator’s intrinsic growth rate, ν is the half saturation constant, d_2 is the diffusion coefficient of the zooplankton, and λ_1 and λ_2 are inertial times for the phytoplankton and the zooplankton, respectively. In this case, the co-existing homogeneous steady-state solution is the point $(u_1^*, u_2^*) \in \mathbb{R}^2$, where the coordinates are defined by

$$u_1^* = \zeta u_2^*, \tag{70}$$

$$u_2^* = \frac{9\zeta - 10 + \sqrt{121\zeta^2 - 180\zeta + 100}}{20\zeta^2}. \tag{71}$$

Example 5.1: In this example, we will let $\psi_{u_1} = \psi_{u_2} \equiv 0$, while ϕ_{u_1} and ϕ_{u_2} will be small positive random perturbations about the steady-state solution. Let us fix the parameters $\theta = 0.25$, $\nu = 0.1$, $d_2 = 25, L = 400$ and $T = 600$. Moreover, for we will consider the weakly hyperbolic case $\lambda_1 = \lambda_2 = 0.001$, and the non-fractional for comparison purposes. Numerically, we let $h = h_{x_1} = h_{x_2} = 1$ and $\tau = 0.01$. Figure 2 shows the results of our simulations in the form of interpolated checkerboard graphs for u_1 (left column) and u_2 (right column) as functions of x_1 and x_2. Various values of ζ were used, namely, $\zeta = 0.28$ (top row), $\zeta = 0.7$ (middle row) and $\zeta = 1.15$ (bottom row). The graphs were obtained using an implementation of (26) to solve the system (69). The results depict the transition between 'cold' and 'hot' spots through labyrinthine structures. This is obviously in agreement with the results on the parabolic model studied in [69]. We have repeated these computational experiments using $\alpha_1 = \alpha_2 = 1.7$ and $\alpha_1 = \alpha_2 = 1.4$. The results are shown in Figures 3 and 4, respectively, and they show the same qualitative behaviour as in the non-fractional scenario of Figure 2. Moreover, note that the patterns are bigger the smaller the values of $\alpha_1 = \alpha_2$. This is in qualitative agreement with the results observed in [45].

It is important to point out that our simulations were able to preserve the positivity and the boundedness of the approximations in all cases. This is in perfect agreement with the fact that the scheme is capable of preserving those features of the relevant solutions. We must mention that we have carried out more computational experiments like those in the previous examples, and we have been able to establish some interesting physical conclusions. For instance, we have noted that the type of Turing patterns present in a weakly hyperbolic system do not depend on the differentiation order, as long as these orders satisfy $\alpha_1 = \alpha_2$ and $\alpha_1, \alpha_2 \in (1, 2]$. Moreover, we have noted that the size of the Turing patterns increase as α_1 and α_2 decrease. Of course, other interesting questions arise. For example, one wonders what are the roles of λ_1 and λ_2 in the presence of complex patterns in the model (69). This and other questions possess physical relevance, but lie outside the scope of the present work. However, they can be tackled numerically using an efficient implementation of our present methodology.

Example 5.2: Figure 5 shows the approximate solution of u_1 in the three-dimensional scenario at the times (a) $t = 1$, (b) $t = 50$, (c) $t = 100$, (d) $t = 200$, (e) $t = 400$ and (f) $t = 600$. We used the same parameters as in Example 5.1, letting $\zeta = 0.7$ and $h_{x_1} = h_{x_2} = h_{x_3} = 4$. Small random nonzero initial velocities were fixed, and the initial profiles were small positive random perturbations about $(0.5, 0.5, 0.5)$. The graphs exhibit the appearance of interesting patterns in a model for which the three-dimensional case has not been studied analytically or numerically. In that sense, the present methodology could be a helpful tool in the investigation of multidimensional systems in the physical sciences.

In the following example, we will confirm numerically the quadratic order of convergence of our numerical scheme. To that end, we will consider the absolute error at the time T between the exact solution u_1 of the continuous model (69) and the corresponding discrete approximations U_1, which is given by

$$\epsilon_{\tau,h} = |||u_1 - U_1|||_\infty. \tag{72}$$

Alternatively, one could use the exact solution u_2 and the respective approximation U_2, but similar results are obtained. To estimate the exact solutions, sufficiently small values of the computational

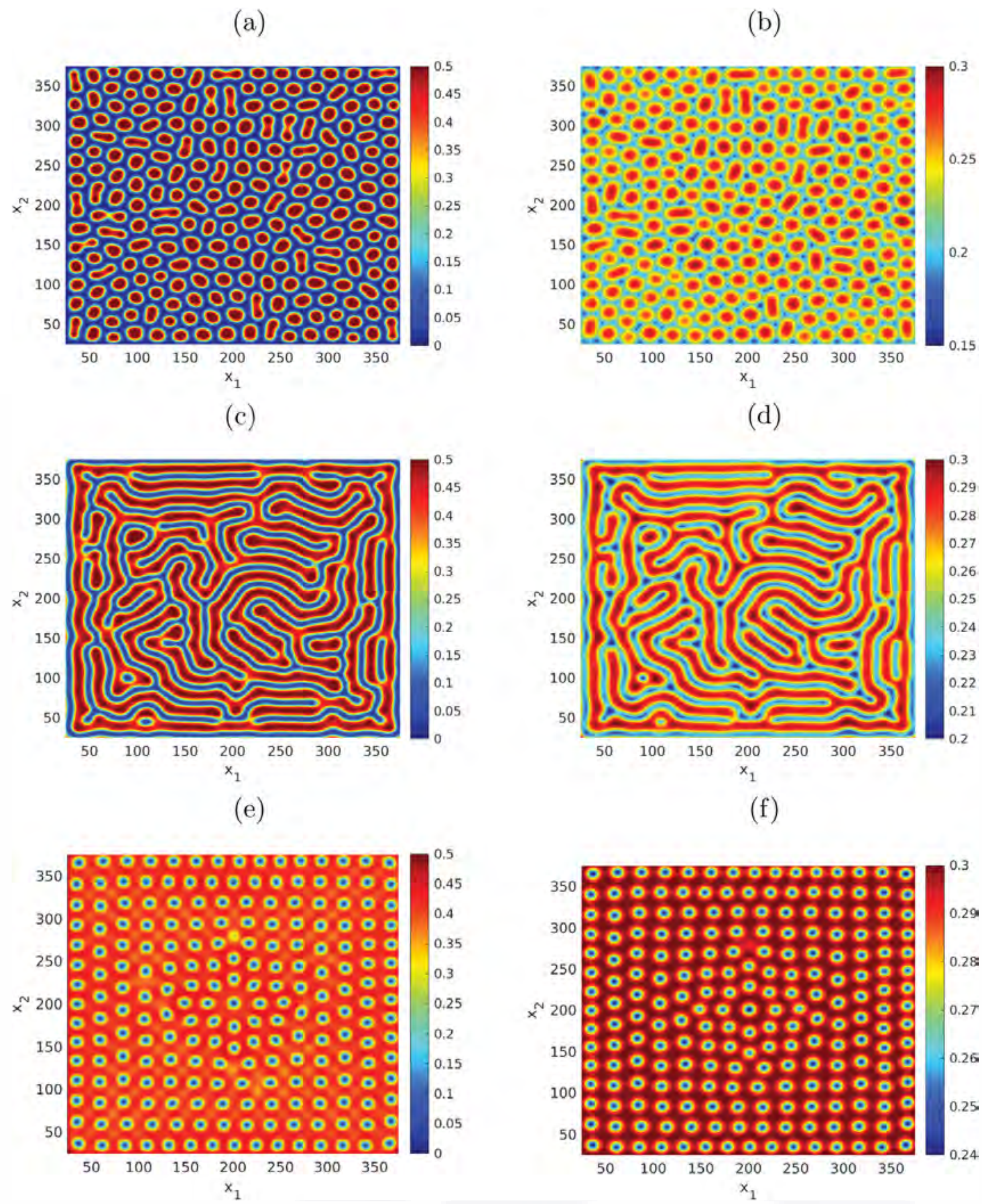

Figure 2. Interpolated checkerboard graphs of the solutions of the system (69) versus $x = (x_1, x_2)$ at the time $T = 600$. The parameters employed are $\theta = 0.25$, $\nu = 0.1$, $d_2 = 25$ and $T = 600$. The weak hyperbolic case $\lambda_1 = \lambda_2 = 0.01$ was considered, in the non-fractional scenario $\alpha_1 = \alpha_2 = 2$. Computationally, we set $h_{x_1} = h_{x_2} = 1$ and $\tau = 0.01$. Small random nonzero initial velocities were fixed, and the initial profiles were small positive random perturbations about the steady-state solution (u_1^*, u_2^*) given by (70)–(71). The graphs correspond to u_1 (left column) and u_2 (right column). Various values of ζ were used, namely, $\zeta = 0.28$ (top row), $\zeta = 0.7$ (middle row) and $\zeta = 1.15$ (bottom row).

parameters are employed to that end. We will also consider the standard rates

$$\rho^t_{\tau,h} = \log_2\left(\frac{\epsilon_{2\tau,h}}{\epsilon_{\tau,h}}\right), \quad \rho^x_{\tau,h} = \log_2\left(\frac{\epsilon_{\tau,2h}}{\epsilon_{\tau,h}}\right). \tag{73}$$

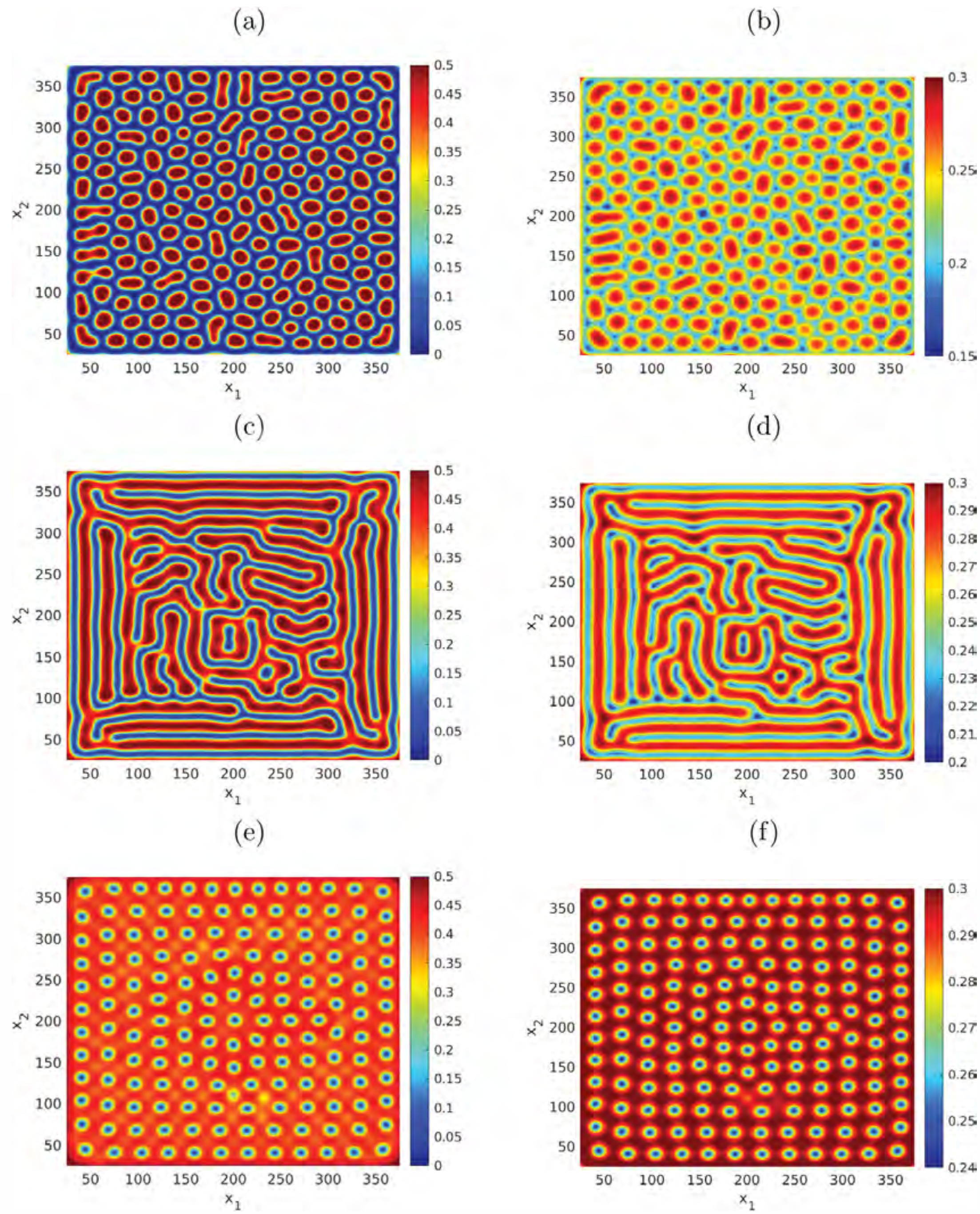

Figure 3. Interpolated checkerboard graphs of the solutions of the system (69) versus $x = (x_1, x_2)$ at the time $T = 600$. The parameters employed are $\theta = 0.25$, $\nu = 0.1$, $d_2 = 25$ and $T = 600$. The weak hyperbolic case $\lambda_1 = \lambda_2 = 0.01$ was considered, in the fractional scenario $\alpha_1 = \alpha_2 = 1.85$. Computationally, we set $h_{x_1} = h_{x_2} = 1$ and $\tau = 0.01$. Small random nonzero initial velocities were fixed, and the initial profiles were small positive random perturbations about the steady-state solution (u_1^*, u_2^*) given by (70)–(71). The graphs correspond to u_1 (left column) and u_2 (right column). Various values of ζ were used, namely, $\zeta = 0.28$ (top row), $\zeta = 0.7$ (middle row) and $\zeta = 1.15$ (bottom row).

Example 5.3: Consider the same set of parameters employed in Example 5.1, using $T= 100$, $\zeta = 0.7$ and $\alpha_1 = \alpha_2 = 1.4$. Under these circumstances, Table 1(a,b) provides, respectively, temporal and spatial analyses of the convergence of the scheme (26). Various values of the computational parameters were considered to obtain the simulations, but all of them establish that the scheme has second order of convergence in both space and time. This is in agreement with the conclusion of Theorem 4.8. It is worth mentioning that the spatial analysis of convergence was performed on the

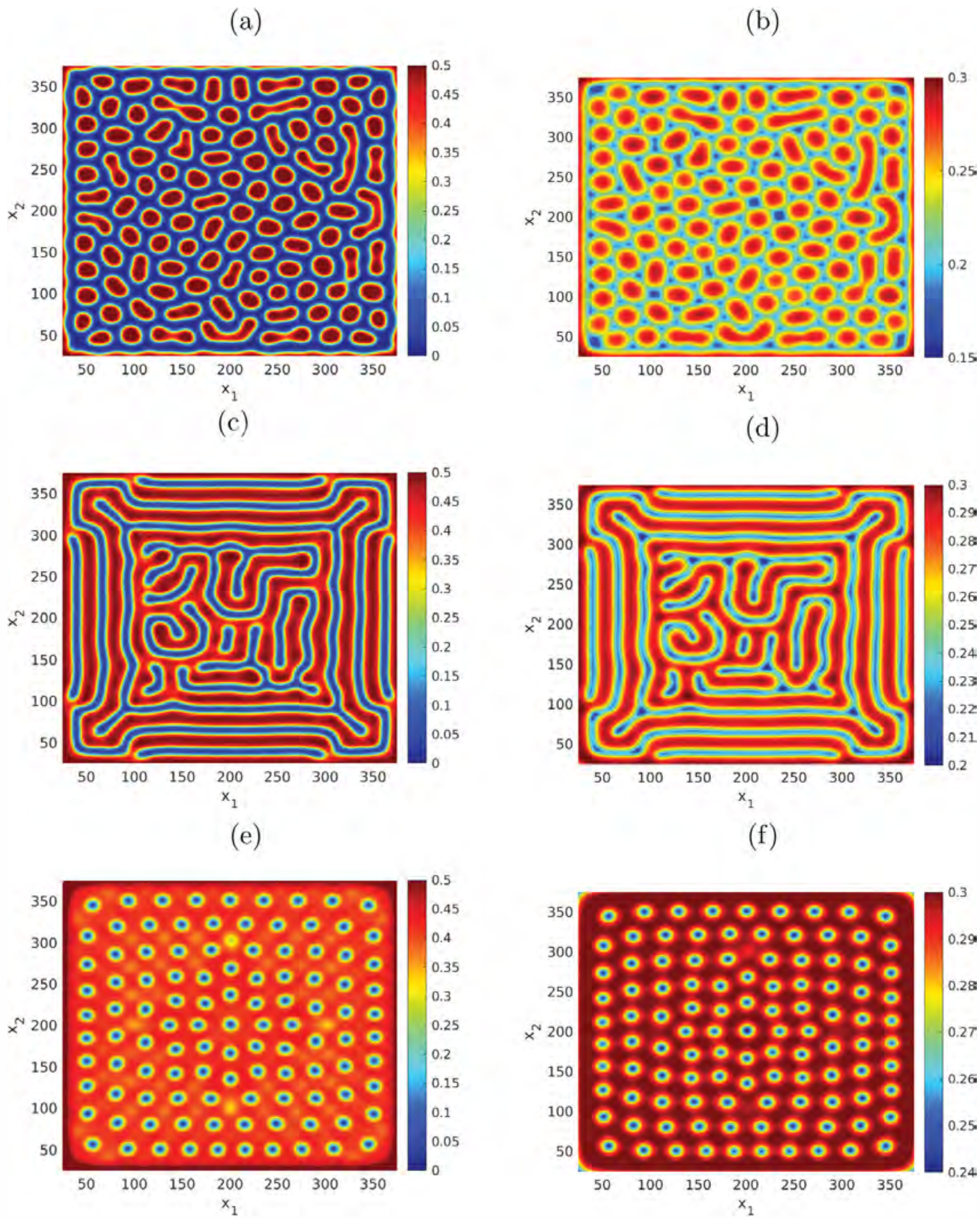

Figure 4. Interpolated checkerboard graphs of the solutions of the system (69) versus $x = (x_1, x_2)$ at the time $T = 600$. The parameters employed are $\theta = 0.25$, $\nu = 0.1$, $d_2 = 25$ and $T = 600$. The weak hyperbolic case $\lambda_1 = \lambda_2 = 0.01$ was considered, in the fractional scenario $\alpha_1 = \alpha_2 = 1.7$. Computationally, we set $h_{x_1} = h_{x_2} = 1$ and $\tau = 0.01$. Small random nonzero initial velocities were fixed, and the initial profiles were small positive random perturbations about the steady-state solution (u_1^*, u_2^*) given by (70)–(71). The graphs correspond to u_1 (left column) and u_2 (right column). Various values of ζ were used, namely, $\zeta = 0.28$ (top row), $\zeta = 0.7$ (middle row) and $\zeta = 1.15$ (bottom row).

parameter h_{x_1}, keeping $h_{x_2} = 2 \times 10^{-2}$ fixed. A similar analysis of convergence on the parameter h_{x_2} was performed, keeping the other spatial step-size fixed. We have not included the results of our simulations to avoid redundancy, but they confirm that the scheme (26) is also quadratically convergent in this computational parameter.

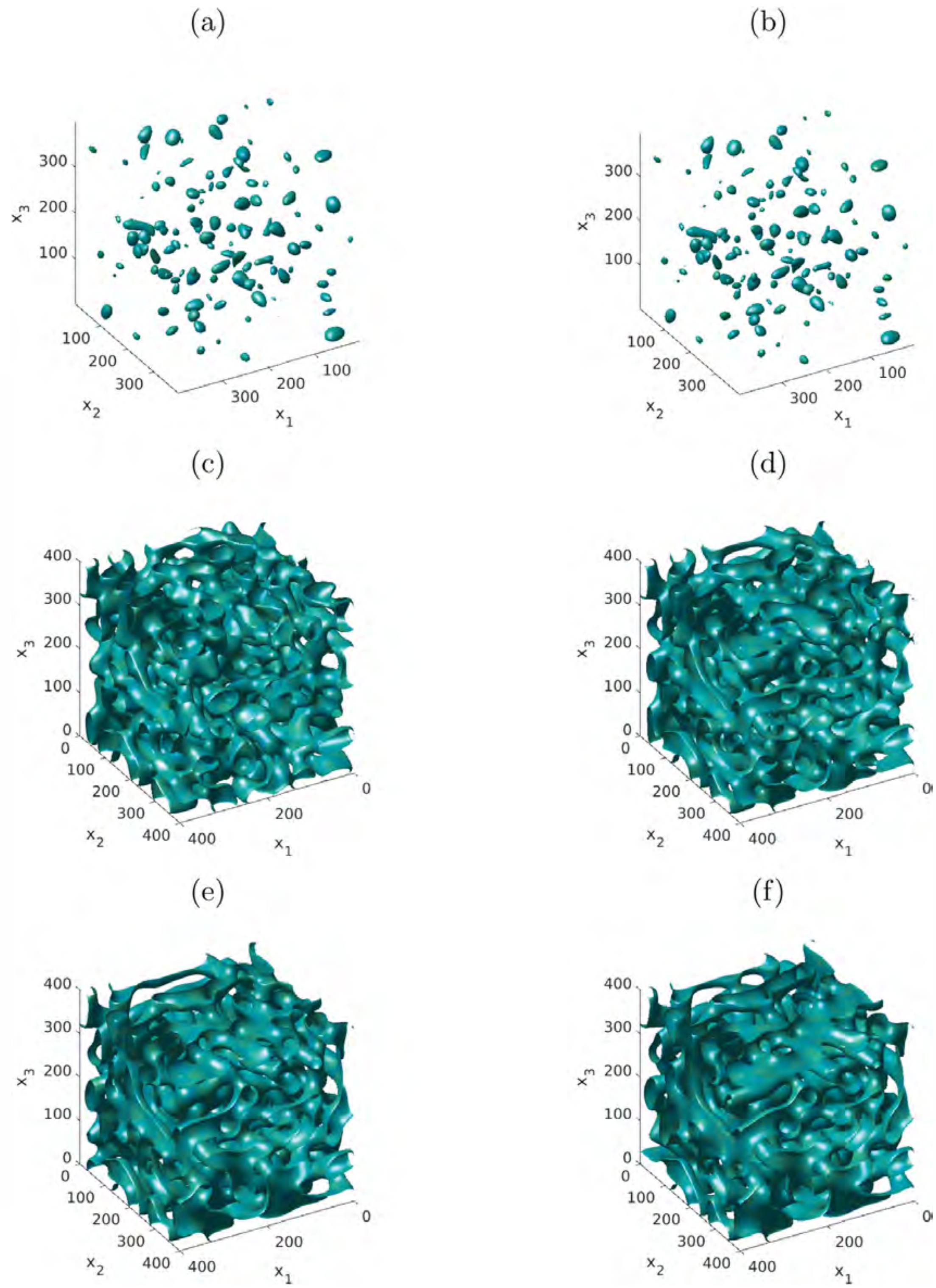

Figure 5. Approximation to the solution u_1 of the system (69) versus $x = (x_1, x_2, x_3)$ at the time $T = 600$. The parameters employed are $\theta = 0.25$, $\nu = 0.1$, $d_2 = 25$ and the times (a) $t = 1$, (b) $t = 50$, (c) $t = 100$, (d) $t = 200$, (e) $t = 400$ and (f) $t = 600$. The weak hyperbolic case $\lambda_1 = \lambda_2 = 0.01$ was considered, in the fractional scenario $\alpha_1 = \alpha_2 = 1.7$ with $\zeta = 0.7$. Computationally, we set $h_{x_1} = h_{x_2} = h_{x_3} = 4$ and $\tau = 0.01$. Small random nonzero initial velocities were fixed, and the initial profiles were small positive random perturbations about $(0.5, 0.5, 0.5)$.

Before closing this section, we must mention that the simulations were obtained in a Dell® Precision T7920 Workstation with Intel® Xeon(R) Gold 5122 CPU @3.60GHz ×16 processor, 125.6 GiB memory, NV137 graphics and disk capacity of 1.0TB. We used 64-bit Fedora 32 (Workstation Edition)

Table 1. Computational studies of (a) temporal and (b) spatial rates of convergence of the finite-difference scheme (26). Various values of the computational parameters were considered in these experiments. The problem under investigation is that described in Example 5.3. The spatial analysis of convergence was performed on the parameter h_{x_1}, fixing $h_{x_2} = 2 \times 10^{-2}$.

(a) Temporal study of convergence

	$h_{x_1} = h_{x_2} = 0.5$		$h_{x_1} = h_{x_2} = 0.25$	
τ	$\epsilon_{\tau,h}$	$\rho^t_{\tau,h}$	$\epsilon_{\tau,h}$	$\rho^t_{\tau,h}$
$0.02/2^0$	2.647307×10^{-4}	–	5.331470×10^{-5}	–
$0.02/2^1$	5.811097×10^{-5}	2.187643	1.027053×10^{-6}	2.376022
$0.02/2^2$	1.103265×10^{-5}	2.397031	1.738615×10^{-6}	2.562501
$0.02/2^3$	2.667038×10^{-6}	2.048469	3.397856×10^{-7}	2.355242
$0.02/2^4$	7.475141×10^{-7}	1.835066	9.079984×10^{-8}	1.903863

(b) Spatial study of convergence

	$\tau = 0.00002$		$\tau = 0.00001$	
h_{x_1}	$\epsilon_{\tau,h}$	$\rho^x_{\tau,h}$	$\epsilon_{\tau,h}$	$\rho^x_{\tau,h}$
$0.5/2^0$	5.278390×10^{-5}	–	1.377958×10^{-5}	–
$0.5/2^1$	1.107331×10^{-5}	2.253011	2.521764×10^{-6}	2.450027
$0.5/2^2$	2.116571×10^{-6}	2.387286	3.9882172×10^{-7}	2.662806
$0.5/2^3$	4.618371×10^{-7}	2.196273	7.601919×10^{-8}	2.389120
$0.5/2^4$	1.125855×10^{-7}	2.036362	1.546677×10^{-8}	2.297191

as the operating system, GNOME version 3.36.3 and Wayland Windowing System. Meanwhile, the implementation of the code was carried out using GFortran and the natively supported library `OpenMP` for parallel computing. To that end, the Fortran 95 implementation of the two- and three-dimensional schemes were proposed in such way that portions of the code were able to be executed in parallel. The results were saved as text files which were later on opened in Matlab®. On the other hand, the graphs were obtained from those text files using standard Matlab® functions.

6. Conclusions

In the present manuscript, we considered a general system of partial differential equations with nonlinear coupled reaction terms. The system considered hyperbolic terms and constant damping coefficients along with fractional diffusion of the Riesz type. The system considered a finite though arbitrary number of spatial coordinates. Also, a finite and arbitrary number of equations was considered herein, making our model sufficiently general to be able to describe various problems from the physical sciences. A structure-preserving finite-difference discretization based on the use of fractional-order centred differences was presented here to solve the continuous model. The scheme is a three-step model, which may be nonlinear depending on the expressions of the reaction terms. Using Brouwer's fixed-point theorem, we established rigorously the existence of solutions of the discrete model. Moreover, we provided sufficient conditions to guarantee the preservation of the positivity and the boundedness of the scheme. In that sense, our numerical technique is a structure-preserving technique which is numerically efficient. Indeed, we proved mathematically that the methodology proposed in this work is consistent of second order in both space and time. Using a discrete form of the energy method, we established the stability of the discrete model along with the second-order convergence in space and time. As a corollary of the stability of our scheme, the uniqueness of the solutions of the method is a straightforward corollary. Some illustrative simulations were provided in order to show the capability of the scheme to reproduce Turing patterns in a hyperbolic reaction-diffusion system. The simulations were obtained through a computer implementation of the discrete model, and they showed that the scheme is capable of preserving both the positivity and the boundedness of approximations. Finally, some numerical experiments showed that the numerical scheme has second order of convergence in both space and time, in agreement with the theoretical results derived in this report. As one of the reviewers pointed out, an approach similar to the present methodology may be employed to investigate various other problems [8–11,58].

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Disclosure statement

No potential conflict of interest was reported by the authors.

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3. A finite-difference discretization preserving the structure of solutions of a diffusive model of type-1 human immunodeficiency virus

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A finite-difference discretization preserving the structure of solutions of a diffusive model of type-1 human immunodeficiency virus

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Abstract

We investigate a model of spatio-temporal spreading of human immunodeficiency virus HIV-1. The mathematical model considers the presence of various components in a human tissue, including the uninfected CD4$^+$T cells density, the density of infected CD4$^+$T cells, and the density of free HIV infection particles in the blood. These three components are nonnegative and bounded variables. By expressing the original model in an equivalent exponential form, we propose a positive and bounded discrete model to estimate the solutions of the continuous system. We establish conditions under which the nonnegative and bounded features of the initial-boundary data are preserved under the scheme. Moreover, we show rigorously that the method is a consistent scheme for the differential model under study, with first and second orders of consistency in time and space, respectively. The scheme is an unconditionally stable and convergent technique which has first and second orders of convergence in time and space, respectively. An application to the spatio-temporal dynamics of HIV-1 is presented in this manuscript. For the sake of reproducibility, we provide a computer implementation of our method at the end of this work.

MSC: Primary 65M06; secondary 65M22; 65Q10

Keywords: Human immunodeficiency virus; Diffusive mathematical model; Structure-preserving finite-difference scheme

1 Introduction

In this manuscript, we agree that a, b, and T^* are real numbers such that $a < b$ and $T^* > 0$. We fix the spatial domain $B = (a,b)$ and the space-time domain $\Omega = B \times (0,T^*)$. The notation $\overline{\Omega}$ is used to denote the closure of the set Ω in the usual topology of $\mathbb{R}^2$, and we use ∂B to represent the boundary of the set B. In this work, we assume that the functions $T, U, V : \overline{\Omega} \to \mathbb{R}$ are sufficiently smooth. Meanwhile, the constants β, d, k, δ, γ, c, and N represent nonnegative numbers. Also, we define the functions $\phi_T, \phi_U, \phi_V : \overline{B} \to \mathbb{R}$ and $\psi_T, \psi_U, \psi_V : \partial B \times [0,T] \to \mathbb{R}$. Assume additionally that $\phi_W(x) = \psi_W(x,0)$ holds for each $x \in \partial B$ and $W \in \{T, U, V\}$.

Table 1 Physical meaning of the parameters in the continuous model (1)

Parameter	Physical meaning
β	New T-cells supply rate
d	Rate of natural death
κ	Rate of infection T-cells
δ	Death rate of infected T-cells
γ	Rate of return of infected cells to uninfected class
c	Clearance rate of the virus
N	Average number of particles infected by infected cells

Under these conventions and nomenclature, the model of type-1 human immunodeficiency virus (HIV-1) infection of CD4⁺T cells with diffusion is described by the one-dimensional problem with initial-boundary conditions:

$$
\begin{aligned}
&\frac{\partial T}{\partial t} = \beta - \kappa VT - dT + \gamma U + \frac{\partial^2 T}{\partial x^2}, \quad \forall (x,t) \in \Omega, \\
&\frac{\partial U}{\partial t} = \kappa VT - (\gamma + \delta)U + \frac{\partial^2 U}{\partial x^2}, \quad \forall (x,t) \in \Omega, \\
&\frac{\partial V}{\partial t} = N\delta U - cV + \frac{\partial^2 V}{\partial x^2}, \quad \forall (x,t) \in \Omega, \\
&\text{such that} \begin{cases} T(x,0) = \phi_T(x), & \forall x \in B, \\ U(x,0) = \phi_U(x), & \forall x \in B, \\ V(x,0) = \phi_V(x), & \forall x \in B, \\ T = \psi_T, \quad U = \psi_U, \quad V = \psi_V, & \forall (x,t) \in \partial B \times [0,T]. \end{cases}
\end{aligned}
\tag{1}
$$

This model is a system with diffusion. The functions $T(x,t)$, $U(x,t)$, and $V(x,t)$ represent the normalized densities of the uninfected CD4⁺T cells, infected CD4⁺T cells, and the free HIV-1 infection particles in the blood, respectively. The physical meanings of the parameters β, d, κ, δ, γ, c, and N are given in Table 1.

In order to express system (1) in an equivalent form, we suppose that T, U, and V are positive solutions of system (1), and let $\lambda \in \mathbb{R}^+$ be a free constant. Dividing both sides of each equation of the population system by $T(x,t) + \lambda$, $U(x,t) + \lambda$, and $V(x,t) + \lambda$, respectively, and using the chain rule at the left-hand side of each equation, we obtain the following equivalent system:

$$
\begin{aligned}
&\frac{\partial}{\partial t} \ln(T + \lambda) = \frac{1}{T + \lambda}\left[\beta - \kappa VT - dT + \gamma U + \frac{\partial^2 T}{\partial x^2}\right], \quad \forall (x,t) \in \Omega, \\
&\frac{\partial}{\partial t} \ln(U + \lambda) = \frac{1}{U + \lambda}\left[\kappa VT - (\gamma + \delta)U + \frac{\partial^2 U}{\partial x^2}\right], \quad \forall (x,t) \in \Omega, \\
&\frac{\partial}{\partial t} \ln(V + \lambda) = \frac{1}{V + \lambda}\left[N\delta U - cV + \frac{\partial^2 V}{\partial x^2}\right], \quad \forall (x,t) \in \Omega, \\
&\text{such that} \begin{cases} T(x,0) = \phi_T(x), & \forall x \in B, \\ U(x,0) = \phi_U(x), & \forall x \in B, \\ V(x,0) = \phi_V(x), & \forall x \in B, \\ T = \psi_T, \quad U = \psi_U, \quad V = \psi_V, & \forall (x,t) \in \partial B \times [0,T]. \end{cases}
\end{aligned}
\tag{2}
$$

This equivalent form is employed to propose an exponential-type discretization of the continuous problem under investigation. In particular, we provide a Bhattacharya-type discrete scheme to solve the mathematical model (2). The reason to follow this approach obeys the need to preserve some important features of the relevant solutions of this system and to provide an unconditionally stable and explicit numerical solution for our differential model.

It is worth pointing out that the mathematical investigation of the human immunodeficiency virus HIV-1 is an interesting avenue of research. In fact, some works investigate mathematical models to estimate HIV-1 virological failure and establish rigorously the role of lymph node drug penetration [1], the global analysis of the dynamics of predictive systems for intermittent HIV-1 treatment [2], mathematical models of cell-wise spread of HIV-1 which include temporal delays [3], models for patterns of the sexual behavior and their relation with the spread of HIV-1 [4], and the long-term dynamics in mathematical models of HIV-1 with temporal delay in various variants of the drug therapy [5]. Some of these models are based on ordinary differential equations, and their analytical study is followed by simulation experiments which assess the validity of the qualitative results. To that end, various numerical methodologies have been designed and analyzed, like some algorithms for simulating the HIV-1 dynamics at a cellular level [6], stem cells therapy of HIV-1 infections [7], fractional optimal control problems on HIV-1 infection of $CD4^{+}T$ cells using Legendre spectral collocation [8], HIV-1 cure models with fractional derivatives which possess a nonsingular kernel [9], stochastic HIV-1/AIDS epidemic models in two-sex populations [10], among other reports [5, 11–13].

Notice that system (2) is an integer-order diffusive extension of some HIV-1 propagation models available in the literature [9, 14]. The use of such a system is due to the current information available of the mechanisms of $CD4^{+}T$ cells and free HIV-1 infection particles in the blood. In our investigation, we propose a two-level finite difference discretization of (2). Our approach hinges on an exponential-type discretization of the mathematical model, and we prove that the numerical model has various numerical and analytical properties which make it a useful research tool in the study of the propagation of HIV-1. For instance, we prove that the scheme is capable of preserving the positivity and boundedness of solutions. This feature is of the utmost importance in view that the variables under investigation are densities [15]. The properties of consistency, stability, and convergence are thoroughly established in this work. In particular, we show that the scheme is unconditionally stable, and that it has first order of convergence in time and second order in space. We provide some simulations to assess the validity of the theoretical results. Moreover, the computer implementation of the scheme used to obtain the simulations is provided in the Appendix at the end of this work.

Before we begin our study, we must mention that the system under investigation (1) has attracted the attention of these authors due to many important reasons. As we pointed out before, the mathematical model is motivated by various particular models available in the literature which do not consider the presence of diffusion. Those systems are described by ordinary differential equations, whence the investigation of their diffusive generalizations is an important topic of research. Indeed, the consideration of a nonconstant diffusion gives rise to a more realistic and complex scenario. Physically and mathematically, the study of (1) would yield more interesting results. From the numerical perspective, it becomes necessary to possess a reliable tool to investigate the solutions of the mathematical model. After the theoretical and computational investigation of the scheme, researchers in the area would possess a means to obtain trustworthy results to propose predictions on the propagation of HIV-1 in the human body.

2 Numerical model

In this stage, we introduce discrete operators to provide a discrete model to approximate the analytical solutions of continuous problem (2). Our approach employs finite differences, and the method to solve the continuous problem is introduced herein. The main structural features of the proposed scheme is rigorously established in the second half of this section.

Let us define the sets $I_q = 1, 2, \ldots, q$ and $\bar{I}_q = \{0\} \cup I_q$ for each $q \in \mathbb{N}$. Let M and K be natural numbers. We define the set $\partial J = \bar{I}_M \cap \partial B$ and consider discrete partitions corresponding to the intervals $[a, b]$ and $[0, T^*]$ as

$$a = x_0 < x_1 < x_2 < \cdots < x_m < \cdots < x_{M-1} < x_M = b, \quad \forall m \in \bar{I}_M, \tag{3}$$

$$0 = t_0 < t_1 < t_2 < \cdots < t_k < \cdots < t_{K-1} < t_K = T^*, \quad \forall k \in \bar{I}_K, \tag{4}$$

respectively. In the first partition, the value x_m is given by $x_m = x_0 + mh$, where $h = (b-a)/M$ for each $m \in \bar{I}_M$. In the second partition, the value of t_k is given by $t_k = k\tau$, where $\tau = T^*/K$ for each $k \in \bar{I}_K$. We use the nomenclatures T_m^k, U_m^k, and V_m^k to denote numerical approximations to the exact solutions T, U, and V, respectively, at the point x_m and time t_k for each $m \in \bar{I}_M$ and $k \in \bar{I}_K$.

Let W be any of T, U, or V. We introduce the following discrete quantities for each $m \in I_{M-1}$ and each $k \in I_{K-1}$:

$$\delta_t W_m^k = \frac{W_m^{k+1} - W_m^k}{\tau}, \tag{5}$$

$$\delta_x^2 W_m^k = \frac{W_{m+1}^k - 2W_m^k + W_{m-1}^k}{h^2}. \tag{6}$$

It is well known that the first operator yields a first-order estimate for the partial derivative of W with respect to t at the point (x_m, t_k), while the second operator yields a second-order estimate of the second partial derivative of W with respect to x at the point (x_m, t_k). Substituting these discrete operators at the time t_k into model (2), we reach the next finite-difference scheme to estimate the solutions of (2) at $(m, k) \in I_{M-1} \times \bar{I}_{K-1}$:

$$\begin{aligned}
\delta_t \ln\left(T_m^k + \lambda\right) &= \frac{1}{T_m^k + \lambda}\left[\beta - \kappa V_m^k T_m^k - dT_m^k + \gamma U_m^k + \delta_x^2 T_m^k\right], \\
\delta_t \ln\left(U_m^k + \lambda\right) &= \frac{1}{U_m^k + \lambda}\left[\kappa V_m^k T_m^k - (\gamma + \delta) U_m^k + \delta_x^2 U_m^k\right], \\
\delta_t \ln\left(V_m^k + \lambda\right) &= \frac{1}{V_m^k + \lambda}\left[N\delta U_m^k - cV_m^k + \delta_x^2 V_m^k\right],
\end{aligned} \tag{7}$$

$$\text{such that}\begin{cases} T_m^0 = \phi_T(x_m), & \forall m \in \bar{I}_M,\\ U_m^0 = \phi_U(x_m), & \forall m \in \bar{I}_M,\\ V_m^0 = \phi_V(x_m), & \forall m \in \bar{I}_M,\\ T_m^k = \psi_T(x_m,t_k), & \forall (m,k) \in \partial J \times \bar{I}_K,\\ U_m^k = \psi_U(x_m,t_k), & \forall (m,k) \in \partial J \times \bar{I}_K,\\ V_m^k = \psi_V(x_m,t_k), & \forall (m,k) \in \partial J \times \bar{I}_K.\end{cases}$$

It is clear that this numerical model is a two-step exponential discretization of the continuous problem (2). Indeed, using the discrete operators, it is an easy algebraic task to check that (7) can be equivalently rewritten as follows:

$$\begin{aligned} T_m^{k+1} &= \left(T_m^k + \lambda\right)\exp\left[\frac{\tau(\beta - (\kappa V_m^k + d + \frac{2}{h^2})T_m^k + \gamma U_m^k + a_{T,m}^k + e_{T,m}^k)}{T_m^k + \lambda}\right] - \lambda,\\ U_m^{k+1} &= \left(U_m^k + \lambda\right)\exp\left[\frac{\tau(\kappa V_m^k T_m^k - (\gamma + \delta + \frac{2}{h^2})U_m^k + a_{U,m}^k + e_{U,m}^k)}{U_m^k + \lambda}\right] - \lambda,\\ V_m^{k+1} &= \left(V_m^k + \lambda\right)\exp\left[\frac{\tau(N\delta U_m^k - (c + \frac{2}{h^2})V_m^k + a_{V,m}^k + e_{V,m}^k)}{V_m^k + \lambda}\right] - \lambda,\\ &\text{such that}\begin{cases} T_m^0 = \phi_T(x_m), & \forall m \in \bar{I}_M,\\ U_m^0 = \phi_U(x_m), & \forall m \in \bar{I}_M,\\ V_m^0 = \phi_V(x_m), & \forall m \in \bar{I}_M,\\ T_m^k = \psi_T(x_m,t_k), & \forall (m,k) \in \partial J \times \bar{I}_K,\\ U_m^k = \psi_U(x_m,t_k), & \forall (m,k) \in \partial J \times \bar{I}_K,\\ V_m^k = \psi_V(x_m,t_k), & \forall (m,k) \in \partial J \times \bar{I}_K,\end{cases}\end{aligned} \tag{8}$$

where $a_{W,m}^k = h^{-2}W_{m+1}^k$ and $e_{W,m}^k = h^{-2}W_{m-1}^k$ for each $m \in I_{M-1}$, each $k \in \bar{I}_{K-1}$, and $W \in \{T,U,V\}$. Notice that each of the three equations in (8) can be expressed as $T_m^{k+1} = F_T(T_m^k)$, $U_m^{k+1} = F_U(U_m^k)$, and $V_m^{k+1} = F_V(V_m^k)$, respectively. Here, the expressions of the functions F_T, F_U, and F_V are as follows:

$$\begin{cases} F_T(w) = g_T(w)\exp(\varphi_T(w)) - \lambda,\\ F_U(w) = g_U(w)\exp(\varphi_U(w)) - \lambda,\\ F_V(w) = g_V(w)\exp(\varphi_V(w)) - \lambda.\end{cases} \tag{9}$$

In turn, each function g_T, g_U, and g_V is given by $g_W(w) = w + \lambda$ with $W \in \{T,U,V\}$, and φ_T, φ_U, φ_V are

$$\varphi_T(w) = \frac{\tau}{w+\lambda}\left(\beta - \left(\kappa V_m^k + d + \frac{2}{h^2}\right)w + \gamma U_m^k + a_{T,m}^k + e_{T,m}^k\right), \tag{10}$$

$$\varphi_U(w) = \frac{\tau}{w+\lambda}\left(\kappa V_m^k T_m^k - \left(\gamma + \delta + \frac{2}{h^2}\right)w + a_{U,m}^k + e_{U,m}^k\right), \tag{11}$$

$$\varphi_V(w) = \frac{\tau}{w+\lambda}\left(N\delta U_m^k - \left(c + \frac{2}{h^2}\right)w + a_{V,m}^k + e_{V,m}^k\right). \tag{12}$$

For convenience, we define the $(M+1)$-dimensional real vectors

$$T^k = (T_0^k, T_1^k, \dots, T_m^k, \dots, T_{M-1}^k, T_M^k), \tag{13}$$

$$U^k = (U_0^k, U_1^k, \dots, U_m^k, \dots, U_{M-1}^k, U_M^k), \tag{14}$$

$$V^k = (V_0^k, V_1^k, \dots, V_m^k, \dots, V_{M-1}^k, V_M^k), \tag{15}$$

for each $k \in \bar{I}_K$. In general, we say that a vector $W \in \mathbb{R}$ is *positive* if all the components are positive. In such a case, we use the notation $W > 0$. We say that W is bounded from above by $s \in \mathbb{R}$ if all the components of W are less that s, in which case we employ the notation $W < s$. Finally, if s is a positive number, then we use $0 < W < s$ to represent that $W > 0$ and $W < s$.

The following results show the existence and uniqueness of the solutions of (8) along with the preservation of the constant solutions.

Theorem 1 (Existence and uniqueness) *Let $k \in \bar{I}_{K-1}$. If $T^k > 0$, $U^k > 0$, $V^k > 0$, and $\lambda > 0$, then the discrete model (8) has a unique solution T^{k+1}, U^{k+1}, and V^{k+1}.*

Proof The numbers $T_m^k + \lambda$, $U_m^k + \lambda$, and $V_m^k + \lambda$ are greater than zero. As a consequence, the real numbers $T_m^{k+1} = F_T(T_m^k)$, $U_m^{k+1} = F_U(U_m^k)$, and $V_m^{k+1} = F_V(V_m^k)$ are defined uniquely, whence the existence and uniqueness readily follow. □

Theorem 2 (Constant solutions) *For each $k \in \bar{I}_K$, let T^k, U^k, and V^k be the zero vectors of dimension $M+1$. Then the sequences $(T^k)_{k=0}^K$, $(U^k)_{k=0}^K$, and $(V^k)_{k=0}^K$ form a solution of model (8) if $\phi_T, \phi_U, \phi_V, \psi_T, \psi_U, \psi_V \equiv 0$ and $\beta = 0$.*

Proof By the hypothesis, the vectors $T^0 = U^0 = V^0 = 0$ satisfy the initial-boundary conditions. Now, if $T^k = U^k = V^k = 0$ for some $k \in \bar{I}_{K-1}$, it is easy to verify that $\varphi_T(0) = \varphi_U(0) = \varphi_V(0) = 0$. This implies in particular that $T_m^{k+1} = F_T(0) = 0$, $U_m^{k+1} = F_U(0) = 0$, and $V_m^{k+1} = F_V(0) = 0$ for each $m \in I_{M-1}$. The conclusion follows using induction. □

The next lemma is an important tool to show the positivity and boundedness of the solutions of the discrete system. The proposition is a result from real analysis, and its proof is established through the mean value theorem.

Lemma 3 *Let $F, g, \varphi : [0,1] \to \mathbb{R}$ be such that $F(w) = g(w)\exp(\varphi(w)) - \lambda$ for each $w \in [0,1]$ and some $\lambda \in \mathbb{R}$. Suppose that g and φ are differential and that, for each $w \in [0,1]$, the inequality*

$$g'(w) + g(w)\varphi'(w) > 0 \tag{16}$$

holds. Then F is an increasing function in $[0,1]$.

Lemma 4 *Let $\lambda > 0$ and $k \in \bar{I}_{K-1}$. Define the following positive constants*:

$$B_T^0 = \beta + \gamma + \left(\kappa + d + \frac{2}{h^2}\right)\lambda + \frac{2}{h^2}, \tag{17}$$

$$B_U^0 = \left(\gamma + \delta + \frac{2}{h^2}\right)\lambda + \kappa + \frac{2}{h^2}, \tag{18}$$

$$B_V^0 = \left(c + \frac{2}{h^2}\right)\lambda + N\delta + \frac{2}{h^2}, \tag{19}$$

and assume that $0 < T^k < 1$, $0 < U^k < 1$, *and* $0 < V^k < 1$. *If the inequalities* $\tau B_T^0 < \lambda$, $\tau B_U^0 < \lambda$, *and* $\tau B_V^0 < \lambda$ *hold, then* $F_T(T_m^k)$, $F_U(U_m^k)$, *and* $F_V(V_m^k)$ *are increasing functions for each* $m \in I_{M-1}$ *and each* $k \in \bar{I}_{K-1}$.

Proof Define $H_W(w) = g'_W(w) + g_W(w)\varphi'_W(w)$ for each $W \in \{T, U, V\}$ and each $w \in [0,1]$. After some algebra, it is possible to see that

$$H_T(w) = \frac{G_T(w)}{w + \lambda}, \quad \forall w \in [0,1], \tag{20}$$

$$H_U(w) = \frac{G_U(w)}{w + \lambda}, \quad \forall w \in [0,1], \tag{21}$$

$$H_V(w) = \frac{G_V(w)}{w + \lambda}, \quad \forall w \in [0,1], \tag{22}$$

where

$$G_T(w) = w + \lambda + \tau\left[\gamma U_m^k + a_{T,m}^k + e_{T,m}^k - \kappa\lambda V_m^k - d\lambda - \frac{2\lambda}{h^2} - \beta\right], \tag{23}$$

$$G_U(w) = w + \lambda - \tau\left[\gamma\lambda + \delta\lambda + \frac{2\lambda}{h^2} + \kappa V_m^k T_m^k + a_{U,m}^k + e_{U,m}^k\right], \tag{24}$$

$$G_V(w) = w + \lambda - \tau\left[c\lambda + \frac{2\lambda}{h^2} + N\delta U_m^k + a_{V,m}^k + e_{V,m}^k\right], \tag{25}$$

for each $w \in [0,1]$. Using Lemma 3, we want to prove that the functions F_T, F_U, and F_V are increasing in $[0,1]$. To that effect, we need to show that the functions H_T, H_U, and H_V are positive on $[0,1]$ or, equivalently, that the functions G_T, G_U, and G_V are positive. Using the hypotheses, note

$$\left|a_{W,m}^k\right| \le \frac{1}{h^2}, \quad \forall W \in \{T, U, V\}, \tag{26}$$

$$\left|e_{W,m}^k\right| \le \frac{1}{h^2}, \quad \forall W \in \{T, U, V\}. \tag{27}$$

As a consequence, observe that $G_W(w) \ge \lambda - \tau B_W^0 > 0$ for each $W \in \{T, U, V\}$ and $w \in [0,1]$. In this way, the functions G_T, G_U, and G_V are positive on $[0,1]$. Using Lemma 3, we conclude that the functions F_T, F_U, and F_V are increasing in the interval $[0,1]$. □

Let $W \in \{T, U, V\}$. In the following, $\mathcal{R}_{\phi_W}$ and $\mathcal{R}_{\psi_W}$ represent the ranges of the functions ϕ_W and ψ_W, respectively, over the interval $[0,1]$.

Theorem 5 (Positivity and boundedness) *Let $\lambda > 0$, and suppose that the following inequalities are satisfied*:

$$\begin{cases} \beta + \gamma < d, \\ \kappa + \delta < \gamma, \\ N\delta < c. \end{cases} \tag{28}$$

Let B_T^0, B_U^0, and B_V^0 be as in Lemma 4, and suppose that $\mathcal{R}_{\phi_W}, \mathcal{R}_{\psi_W} \subseteq (0,1)$. If the inequalities $\tau B_T^0 < \lambda$, $\tau B_U^0 < \lambda$, and $\tau B_V^0 < \lambda$ hold, then there are unique sequences of vectors $(T^k)_{k=0}^K$, $(U^k)_{k=0}^K$, and $(V^k)_{k=0}^K$ that satisfy $0 < T^k < 1$, $0 < U^k < 1$, and $0 < V^k < 1$ for each $k \in \bar{I}_K$.

Proof We use induction to reach the conclusion. By hypothesis, the conclusion of this theorem is satisfied for $k = 0$, so let us assume that it holds also for some $k \in \bar{I}_{K-1}$. Lemma 3 assures that the functions F_T, F_U, and F_V are increasing on $[0,1]$. Let $m \in I_{K-1}$. If $\beta = 0$ and $T_m^k = U_m^k = V_m^k = 0$, then it follows that

$$F_T(0) = \lambda \exp\left(\frac{\tau}{\lambda}\left(\beta + \gamma U_m^k\right)\right) - \lambda = 0, \tag{29}$$

$$F_U(0) = \lambda \exp\left(\frac{\tau}{\lambda}\left(\kappa V_m^k T_m^k\right)\right) - \lambda = 0, \tag{30}$$

$$F_V(0) = \lambda \exp\left(\frac{\tau}{\lambda}\left(N\delta U_m^k\right)\right) - \lambda = 0. \tag{31}$$

On the other hand, the hypothesis establishes that

$$\varphi_T(1) < \frac{\tau}{1+\lambda}(\beta - d + \gamma) < 0, \tag{32}$$

$$\varphi_U(1) < \frac{\tau}{1+\lambda}(\kappa - \gamma + \delta) < 0, \tag{33}$$

$$\varphi_V(1) < \frac{\tau}{1+\lambda}(N\delta - c) < 0. \tag{34}$$

This and (9) show that $F_T(1) < 1$, $F_U(1) < 1$, and $F_V(1) < 1$. Notice that the functions $F_T, F_U, F_V : [0,1] \to \mathbb{R}$ are increasing and that $0 < F_W(0) < F_W(1) < 1$ for each $W \in \{T, U, V\}$. The inequalities $0 < W^k < 1$ for $W = T, U, V$ imply that $T_m^{k+1} = F_T(T_m^k)$, $U_m^{k+1} = F_U(U_m^k)$, and $V_m^{k+1} = F_V(V_m^k)$ all are numbers in the set $(0,1)$ for each $m \in I_{M-1}$. Using the data at the boundary, we reach $0 < T_m^{k+1} < 1$, $0 < U_m^{k+1} < 1$, and $0 < V_m^{k+1} < 1$. The conclusion follows using induction. □

As a conclusion of this section, the numerical methodology is a structure-preserving scheme to approximate the solutions of (2). In this manuscript, the concept of 'structure preservation' or 'dynamical consistency' refers not only to the capacity of discrete models to keep discrete versions of some physical features. In this context, these notions refer also to the capability of a numerical method to be able to conserve some mathematical characteristics of the solutions of interest of continuous paradigms, like positivity [16], boundedness [17, 18], monotonicity [19], and convexity of approximations [20], among other physically relevant features [21].

3 Numerical properties

In this stage, we present the main numerical features of the finite-differences scheme (8). More precisely, we are interested in proving consistency, unconditional stability, and convergence. To show the consistency of the numerical scheme, we require the following continuous operators:

$$\mathcal{L}_T T = (T+\lambda)\frac{\partial}{\partial t}\ln(T+\lambda) - \beta + \kappa VT + dT - \gamma U - \frac{\partial^2 T}{\partial x^2}, \tag{35}$$

$$\mathcal{L}_U U = (U+\lambda)\frac{\partial}{\partial t}\ln(U+\lambda) - \kappa VT + (\gamma+\delta)U - \frac{\partial^2 U}{\partial x^2}, \tag{36}$$

$$\mathcal{L}_V V = (V+\lambda)\frac{\partial}{\partial t}\ln(V+\lambda) - N\delta U + cV - \frac{\partial^2 V}{\partial x^2} \tag{37}$$

for each $(x,t) \in \Omega$. Also, we define the difference operators

$$L_T T(x_m,t_k) = \left(T_m^k+\lambda\right)\delta_t \ln\left(T_m^k+\lambda\right) - \beta + \left(\kappa V_m^k + d - \delta_x^2\right)T_m^k - \gamma U_m^k, \tag{38}$$

$$L_U U(x_m,t_k) = \left(U_m^k+\lambda\right)\delta_t \ln\left(U_m^k+\lambda\right) - \kappa V_m^k T_m^k + (\gamma+\delta)U_m^k - \delta_x^2 U_m^k, \tag{39}$$

$$L_V V(x_m,t_k) = \left(V_m^k+\lambda\right)\delta_t \ln\left(V_m^k+\lambda\right) - N\delta U_m^k + cV_m^k - \delta_x^2 V_m^k \tag{40}$$

for each $m \in I_{M-1}$ and $k \in \bar{I}_{K-1}$. For the remainder, the symbols $\|\cdot\|_2$ and $\|\cdot\|_\infty$ are used to denote the Euclidean and the maximum norms in $\mathbb{R}^{M+1}$, respectively.

Theorem 6 (Consistency) *If $T,U,V \in \mathcal{C}^{4,3}_{x,t}(\overline{\Omega})$ and $\lambda > 0$, then there exist positive constants C_T, C_U, and C_V, which are independent of τ and h, such that*

$$\left|\mathcal{L}_W W(x,t) - L_W W(x_m,t_k)\right| \le C_W\left(\tau + h^2\right) \tag{41}$$

for each $m \in I_{M-1}$, $k \in \bar{I}_{K-1}$, and $W \in \{T,U,V\}$.

Proof We prove the consistency only for $W = T$, the consistencies for $W = U$ and $W = V$ are proved in a similar fashion. To that end, we employ the usual arguments based on Taylor polynomials. As a consequence of the hypotheses on the regularity of T, there exist positive constants $C_{T,1}$ and $C_{T,2}$ independent of τ and h such that, for each $(m,k) \in I_{M-1} \times \bar{I}_{K-1}$,

$$\left|\left(T_m^k+\lambda\right)\frac{\partial}{\partial t}\ln\left(T_m^k+\lambda\right) - \left(T_m^k+\lambda\right)\delta_t\ln\left(T_m^k+\lambda\right)\right| \le C_{T,1}\tau, \tag{42}$$

$$\left|\frac{\partial^2 T}{\partial x^2}(x_m,t_k) - \delta_x^2 T_m^k\right| \le C_{T,2}h^2. \tag{43}$$

On the other hand, observe that

$$\left|\kappa V(x_m,t_k)T(x_m,t_k) + dT(x_m,t_k) - \kappa V_m^k T_m^k - dT_m^k\right| = 0, \tag{44}$$

$$\left|\gamma U(x_m,t_k) - \gamma U_m^k\right| = 0. \tag{45}$$

Finally, the conclusion follows now from the triangle inequality after we define the positive constant $C_T = \max\{C_{T,1}, C_{T,2}\}$, which is independent of τ and h. Similarly, we may show the inequalities corresponding to $W = U$ and $W = V$. □

Under the assumptions of this theorem, there is a positive constant C which is independent of τ and h with the property that, for each $m \in I_{M-1}$, $k \in \bar{I}_{K-1}$, and $W \in \{T, U, V\}$,

$$\left|\mathcal{L}_W W(x,t) - L_W W(x_m, t_k)\right| \leq C\left(\tau + h^2\right). \tag{46}$$

Indeed, observe that $C = C_T \vee C_U \vee C_V$ is a constant which satisfies this inequality. This fact will be employed when we prove the convergence of scheme (7). In our next step, we show the stability of the proposed scheme. To that end, we fix two systems of initial-boundary data which are labeled $\Phi = (\phi_T, \phi_U, \phi_V, \psi_T, \psi_U, \psi_V)$ and $\widetilde{\Phi} = (\widetilde{\phi}_T, \widetilde{\phi}_U, \widetilde{\phi}_V, \widetilde{\psi}_T, \widetilde{\psi}_U, \widetilde{\psi}_V)$. The corresponding solutions of (7) are represented respectively by (T, U, V) and $(\widetilde{T}, \widetilde{U}, \widetilde{V})$. In particular, notice that the following result proves that the scheme is unconditionally stable.

Theorem 7 (Stability) *Let Φ and $\widetilde{\Phi}$ be two sets of initial-boundary conditions for problem* (7), *and let $\lambda > 0$. Suppose that the hypotheses of Theorem* 5 *are satisfied for both triplets (T, U, V) and $(\widetilde{T}, \widetilde{U}, \widetilde{V})$. There is a constant C, which is independent of the initial data such that*

$$\left\| W^k - \widetilde{W}^k \right\|_\infty \leq C \left\| W^0 - \widetilde{W}^0 \right\|_\infty, \quad \forall k \in \bar{I}_K, \forall W \in \{T, U, V\}. \tag{47}$$

Proof Beforehand, notice that Theorem 5 guarantees that (T, U, V) and $(\widetilde{T}, \widetilde{U}, \widetilde{V})$ exist and that they are bounded. On the other hand, let $W = T$ and introduce the function $\Phi_m^k : [0,1]^{(M+1)} \to \mathbb{R}$ for each $m \in I_{M-1}$ and $\bar{I}_{K-1}$ by

$$\Phi_m^k(T) = \left(T_m^k + \lambda\right) \exp\left(\frac{\tau \Psi(T)}{T_m^k + \lambda}\right) - \lambda, \quad \forall T \in [0,1]^{(M+1)}. \tag{48}$$

Here, the function $\Psi(T)$ is defined by

$$\Psi(T) = \beta - \left(\kappa V_m^k + d + \frac{2}{h^2}\right) T_m^k + \gamma U_m^k + a_{T,m}^k + e_{T,m}^k. \tag{49}$$

It is readily checked that the function Φ_m^k is of class $\mathcal{C}^1([0,1]^{(M+1)})$ for each $k \in \bar{I}_K$. As a consequence of this, the number $C_{m,k} = \max_{[0,1]^{(M+1)}} \|\nabla \Phi_m^k\|_2$ exists. For each $T, \widetilde{T} \in [0,1]^{(M+1)}$, there exists some $\xi \in [0,1]^{(M+1)}$ with the property that

$$\left|\Phi_m^k(T) - \Phi_m^k(\widetilde{T})\right| \leq \left\|\nabla \Phi_m^k(\xi)\right\|_2 \|T - \widetilde{T}\|_2 \leq C_{m,k}\sqrt{(M+1)}\|T - \widetilde{T}\|_\infty. \tag{50}$$

As consequence, note that, for each $m \in I_{M-1}$,

$$\left|T_m^k - \widetilde{T}_m^k\right| = \left|\Phi_m^k(T) - \Phi_m^k(\widetilde{T})\right| \leq C_k \left\|T^k - \widetilde{T}^k\right\|_\infty, \tag{51}$$

where

$$C_k = 1 \vee \max\left\{C_{m,k}\sqrt{(M+1)} : 1 \leq m \leq M-1\right\}. \tag{52}$$

Using (51), it is clear that $\|T^{k+1} - \widetilde{T}^{k+1}\|_\infty \leq C_k \|T^k - \widetilde{T}^k\|_\infty$ for each $k \in \bar{I}_{K+1}$. Finally, recursion shows now that the inequality $\|T^k - \widetilde{T}^k\|_\infty \leq C_T \|T^0 - \widetilde{T}^0\|_\infty$ is satisfied for each

$k \in \bar{I}_K$, where

$$C_T = (M+1)^{K/2} \prod_{k=0}^{K-1} C_k. \tag{53}$$

Similarly, we can prove that there exist positive constants C_U and C_W, with the property that $\|U^k - \widetilde{U}^k\|_\infty \le C_U \|U^0 - \widetilde{U}^0\|_\infty$ and $\|V^k - \widetilde{V}^k\|_\infty \le C_V \|V^0 - \widetilde{V}^0\|_\infty$. The conclusion is reached now if we define $C = C_T \vee C_U \vee C_V$. □

Finally, we study the convergence of the numerical scheme (8). In the next result, we let (T, U, V) be a solution of differential problem (2) associated with the set of initial-boundary data $\Phi = (\phi_T, \phi_U, \phi_V, \psi_T, \psi_U, \psi_V)$. Meanwhile, the numerical solution obtained through the discrete model (8) is denoted by $(\widetilde{T}, \widetilde{U}, \widetilde{V})$.

Theorem 8 (Convergence) *Let Φ be a set of initial-boundary data which are bounded in* $(0,1)$, *and let* $\lambda > 0$. *Assume that problem* (2) *has a unique solution bounded in* $(0,1)$ *such that* $T, U, V \in \mathcal{C}^{4,3}_{x,t}(\overline{\Omega})$. *Suppose that the conditions of Theorem 5 hold, and let*

$$\exp(\tau/\lambda) - 1 \le 2\tau/\lambda. \tag{54}$$

For each $W = T, U, V$, there is a constant C_W independent of τ and h such that, for each $k \in \bar{I}_K$,

$$\left\| W^k - \widetilde{W}^k \right\|_\infty \le C_W\left(\tau + h^2\right). \tag{55}$$

Proof Beforehand, notice that Theorem 5 assures that positive and bounded solutions for discrete problem (7) exist. Without loss of generality, let $W = T$ and define the difference $e^k_m = T^k_m - \widetilde{T}^k_m$ for each $m \in \bar{I}_M$ and $k \in \bar{I}_K$. Notice that the exact solution T of problem (1) satisfies scheme (8) at the point (x_m, t_k) having some local truncation error R^k_m for each $m \in \bar{I}_{M-1}$ and $k \in \bar{I}_{K-1}$. Also, for each $m \in \bar{I}_{M-1}$ and $k \in \bar{I}_{K-1}$, the analytical and discrete solutions satisfy, respectively,

$$\left(W^k_m + \lambda\right) L_T T^k_m = R^k_m, \tag{56}$$

$$\left(\widetilde{T}^k_m + \lambda\right) L_T \widetilde{T}^k_m = 0. \tag{57}$$

By Theorem (6), there exists $C_0 > 0$ such that $|R^k_m| \le C_0(\tau + h^2)$ for each $m \in \bar{I}_{M-1}$ and $k \in \bar{I}_{K-1}$. Using the definitions of the discrete operators in equations (56) and (57), we have that

$$T^{k+1}_m = \left(T^k_m + \lambda\right) \exp\left(\frac{\tau R^k_m}{T^k_m + \lambda}\right) \exp\left(\varphi_T\left(T^k_m\right)\right) - \lambda, \tag{58}$$

$$\widetilde{T}^{k+1}_m = \left(\widetilde{T}^k_m + \lambda\right) \exp\left(\varphi_T\left(\widetilde{T}^k_m\right)\right) - \lambda \tag{59}$$

for each $m \in \bar{I}_{M-1}$ and $k \in \bar{I}_{K-1}$. Subtracting $\widetilde{T}^k_m$ of T^k_m, we have

$$\begin{aligned}
|e^k_m| &\leq (T^k_m + \lambda) \exp\left[\left(\frac{\tau R^k_m}{T^k_m + \lambda}\right) - 1\right] \exp(\varphi_T(T^k_m)) + |\Phi^k_m(T) - \Phi^k_m(\widetilde{T})| \\
&\leq (1+\lambda) D^k_m [\exp(\tau R^k_m / \lambda) - 1] + C^k_m \|T^k - \widetilde{T}^k\|_\infty \\
&\leq D \tau R^k_m + C\|e^k\|_\infty,
\end{aligned} \tag{60}$$

where

$$e^k = (e^k_0, e^k_1, e^k_2, \ldots, e^k_{M-1}, e^k_M), \tag{61}$$

$$D^k_m = \max\{\exp(\varphi_T(T^k_m)) : T \in [0,1]^{M+1}\} \tag{62}$$

for each $m \in \bar{I}_{M-1}$ and $k \in \bar{I}_{K-1}$. In addition, we let

$$C = \max\{C^k_m \sqrt{M+1} : m = 1, \ldots, M-1; k = 1, \ldots, K-1\}, \tag{63}$$

$$D = \max\left\{\frac{2(1+\lambda)D^k_m}{\lambda} : m = 1, \ldots, M-1; k = 1, \ldots, K-1\right\}. \tag{64}$$

The constants Φ^k_m and C^k_m are as in the proof of Theorem 7. Moreover, all the constants C^k_m are in the interval $[0,1]$, therefore C is an element of the interval $[0,1]$. Theorem 6 implies now that, for each $k \in \bar{I}_{K-1}$,

$$\|e^{k+1}\|_\infty - \|e^k\|_\infty \leq \|e^{k+1}\|_\infty - C\|e^k\|_\infty \leq C_0 D\tau(\tau + h^2). \tag{65}$$

Taking the sum on both ends of the previous inequality and using the initial data, we have

$$\|e^{l+1}\|_\infty = \|e^{l+1}\|_\infty - \|e^0\|_\infty \leq C_0 D T^*(\tau + h^2) = C_T(\tau + h^2), \tag{66}$$

where $l \in \bar{I}_{K-1}$ and $C_T = C_0 D T^*$. The conclusion of this result has been reached now when $W = T$. Analogously, we may easily prove the inequality of the conclusion when $W = U$ and $W = V$. □

4 Application

In this section, we show some computer simulations obtained using the finite-difference scheme (8). Beforehand, notice that the discrete model is an explicit scheme. To describe its computational implementation, for each $k \in \bar{I}_{K+1}$, we redefine the real vectors T^k, U^k, and V^k as follows:

$$T^k = (T^k_1, T^k_2, \ldots, T^k_{M-2}, T^k_{M-1}), \tag{67}$$

$$U^k = (U^k_1, U^k_2, \ldots, U^k_{M-2}, U^k_{M-1}), \tag{68}$$

$$V^k = (V^k_1, V^k_2, \ldots, V^k_{M-2}, V^k_{M-1}). \tag{69}$$

These vectors belong to the set $\mathbb{R}^{M+1}_+$, where $\mathbb{R}_+$ is the system of positive numbers. Also, we define the vectors of initial conditions $\boldsymbol{\phi}_{\mathbf{T}}, \boldsymbol{\phi}_{\mathbf{U}}, \boldsymbol{\phi}_{\mathbf{V}} \in \mathbb{R}^{M-1}_+$ as follows:

$$\boldsymbol{\phi}_{\mathbf{T}} = (\phi_T(x_1), \phi_T(x_2), \ldots, \phi_T(x_{M-2}), \phi_T(x_{M-1})), \tag{70}$$

$$\boldsymbol{\phi}_{\mathbf{U}} = \big(\phi_U(x_1), \phi_U(x_2), \ldots, \phi_U(x_{M-2}), \phi_U(x_{M-1})\big), \tag{71}$$

$$\boldsymbol{\phi}_{\mathbf{V}} = \big(\phi_V(x_1), \phi_V(x_2), \ldots, \phi_V(x_{M-2}), \phi_V(x_{M-1})\big). \tag{72}$$

Meanwhile, for each $k \in \bar{I}_K$, we define the vectors $\boldsymbol{\psi}_{\mathbf{T}}^k, \boldsymbol{\psi}_{\mathbf{U}}^k, \boldsymbol{\psi}_{\mathbf{V}}^k \in \mathbb{R}_+^{M+1}$ of the boundary conditions through

$$\boldsymbol{\psi}_{\mathbf{T}}^k = \big(\psi_T(x_0, t_k), 0, \ldots, 0, \psi_T(x_M, t_k)\big), \tag{73}$$

$$\boldsymbol{\psi}_{\mathbf{U}}^k = \big(\psi_U(x_0, t_k), 0, \ldots, 0, \psi_U(x_M, t_k)\big), \tag{74}$$

$$\boldsymbol{\psi}_{\mathbf{V}}^k = \big(\psi_V(x_0, t_k), 0, \ldots, 0, \psi_V(x_M, t_k)\big). \tag{75}$$

With the previous definitions and for each $k \in \bar{I}_K$, we express the discrete model (8) in vector form as follows:

$$\begin{aligned}
T^{k+1} &= \big(T^k + \lambda\big) \exp\left[\frac{\tau(\beta - (\kappa V^k + d + \frac{2}{h^2})T^k + \gamma U^k + a_T^k + e_T^k)}{T^k + \lambda}\right] - \lambda, \\
U^{k+1} &= \big(U^k + \lambda\big) \exp\left[\frac{\tau(\kappa V^k T^k - (\gamma + \delta + \frac{2}{h^2})U^k + a_U^k + e_U^k)}{U^k + \lambda}\right] - \lambda, \\
V^{k+1} &= \big(V^k + \lambda\big) \exp\left[\frac{\tau(N\delta U^k - (c + \frac{2}{h^2})V^k + a_V^k + e_V^k)}{V^k + \lambda}\right] - \lambda \\
&\text{such that } \begin{cases} T^0 = \boldsymbol{\phi}_{\mathbf{T}}, \\ U^0 = \boldsymbol{\phi}_{\mathbf{U}}, \\ V^0 = \boldsymbol{\phi}_{\mathbf{V}}. \end{cases}
\end{aligned} \tag{76}$$

For each $k \in \bar{I}_K$ and $W \in \{T, U, V\}$, the vectors a_W^k and e_W^k are defined as follows:

$$a_W^k = \frac{1}{h^2}\big(W_2^k, W_3^k, \ldots, W_{M-1}^k, W_M^k\big), \tag{77}$$

$$e_W^k = \frac{1}{h^2}\big(W_0^k, W_1^k, \ldots, W_{M-3}^k, W_{M-2}^k\big). \tag{78}$$

Using the boundary conditions, we readily have that $W_M^k = \psi_W(x_M, t_k)$ and $W_0^k = \psi_W(x_0, t_k)$ for each $k \in \bar{I}_{K+1}$ and $W \in \{T, U, V\}$. So, for all $k \in \bar{I}_K$, the vector form of the finite-difference scheme (8) is defined as follows:

$$\mathbf{T}^k = \big(\psi_T(x_0, t_k), T_1^k, T_2^k, \ldots, T_{M-2}^k, T_{M-1}^k, \psi_T(x_M, t_k)\big), \tag{79}$$

$$\mathbf{U}^k = \big(\psi_U(x_0, t_k), U_1^k, T_2^k, \ldots, U_{M-2}^k, U_{M-1}^k, \psi_U(x_M, t_k)\big), \tag{80}$$

$$\mathbf{V}^k = \big(\psi_V(x_0, t_k), V_1^k, T_2^k, \ldots, V_{M-2}^k, V_{M-1}^k, \psi_V(x_M, t_k)\big). \tag{81}$$

The next experiments employ variations of the computer code in the Appendix, which is a basic computational implementation of our finite-difference scheme. The parameter values and the type of initial conditions are motivated by data used in the literature for similar models but without diffusion [9, 14].

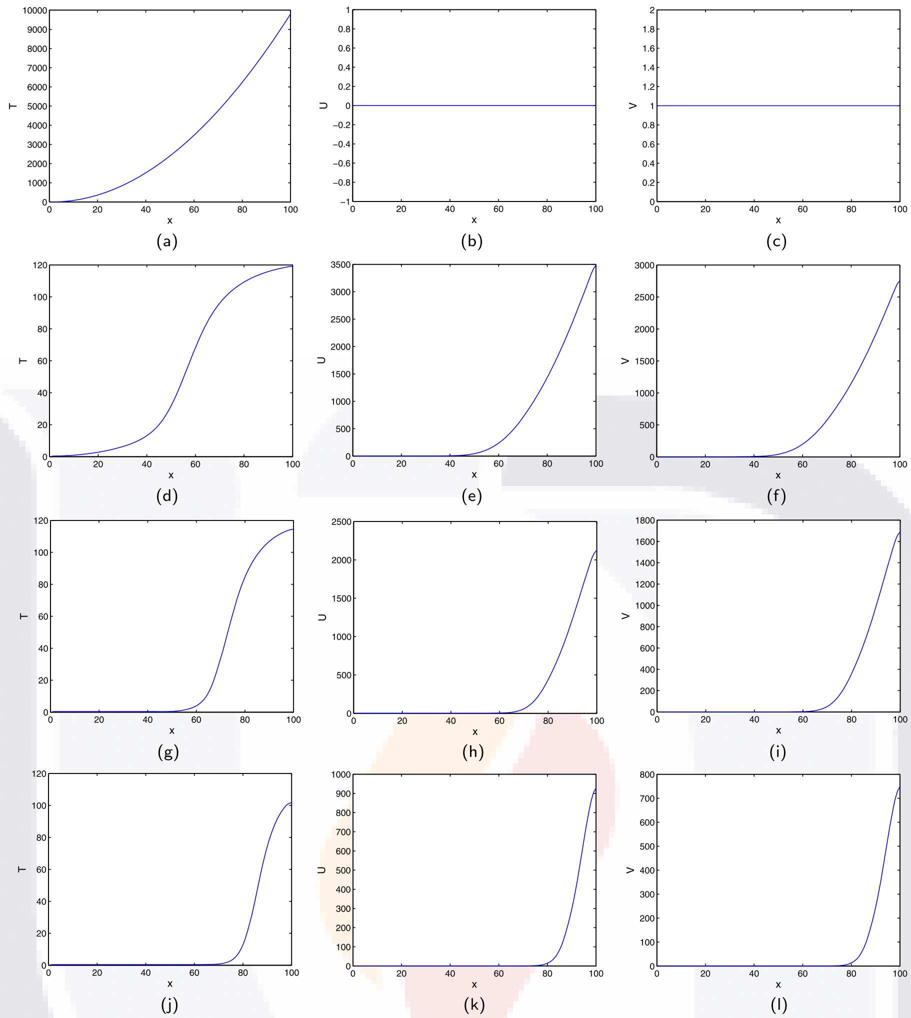

Figure 1 Snapshots of the approximate solutions T, U, and V of (1) for each row at the time $t = 0$, $t = 1$, $t = 3$, and $t = 5$. The parameters employed are $\lambda = 0.1$, $\beta = 2$, $d = 5.05$, $\kappa = 0.03$, $\delta = 0.016$, $\gamma = 3.0$, $c = 20.4$, and $N = 1000$. We let $\phi_T(x)$, $\phi_U(x)$, and $\phi_V(x)$ be as in Example 9. The approximations were calculated using our implementation of (76) in the Appendix, with $\tau = 0.00001$ and $h = 1$

Example 9 In this example, we let $B = (0, 100)$ and define the initial conditions ϕ_T, ϕ_U, and ϕ_V as $\phi_T(x) = x^2$, $\phi_U(x) = 0$, and $\phi_V(x) = 1$ for each $x \in B$. These initial data describe an initial state in which no infected CD4$^+$T cells are present, and the entire medium is formed from free HIV-1 infection particles. In turn, the normal density of the uninfected CD4$^+$T cells increases in the linear medium considered herein. Let $\lambda = 0.1$, $\beta = 2$, $d = 5.05$, $\kappa = 0.03$, $\delta = 0.016$, $\gamma = 3.0$, $c = 20.4$, and $N = 1000$. Under this situation, Fig. 1 provides snapshots of the normalized solutions T, U, and V at the times $t = 0$, $t = 1$, $t = 3$, and $t = 5$. The graphs show that the solutions are positive and bounded in accordance with the results obtained in the previous sections. In our simulations, we used the following computational parameters $\tau = 0.00001$ and $h = 1$.

Example 10 Let $B = (0, 100)$ be as in the previous example, and use the initial conditions $\phi_T(x) = -x^2 + 100x$, $\phi_U(x) = 0$, and $\phi_V(x) = 1$ for each $x \in B$. Set the model and computational parameter values as before. Under these circumstances, Fig. 2 provides snapshots

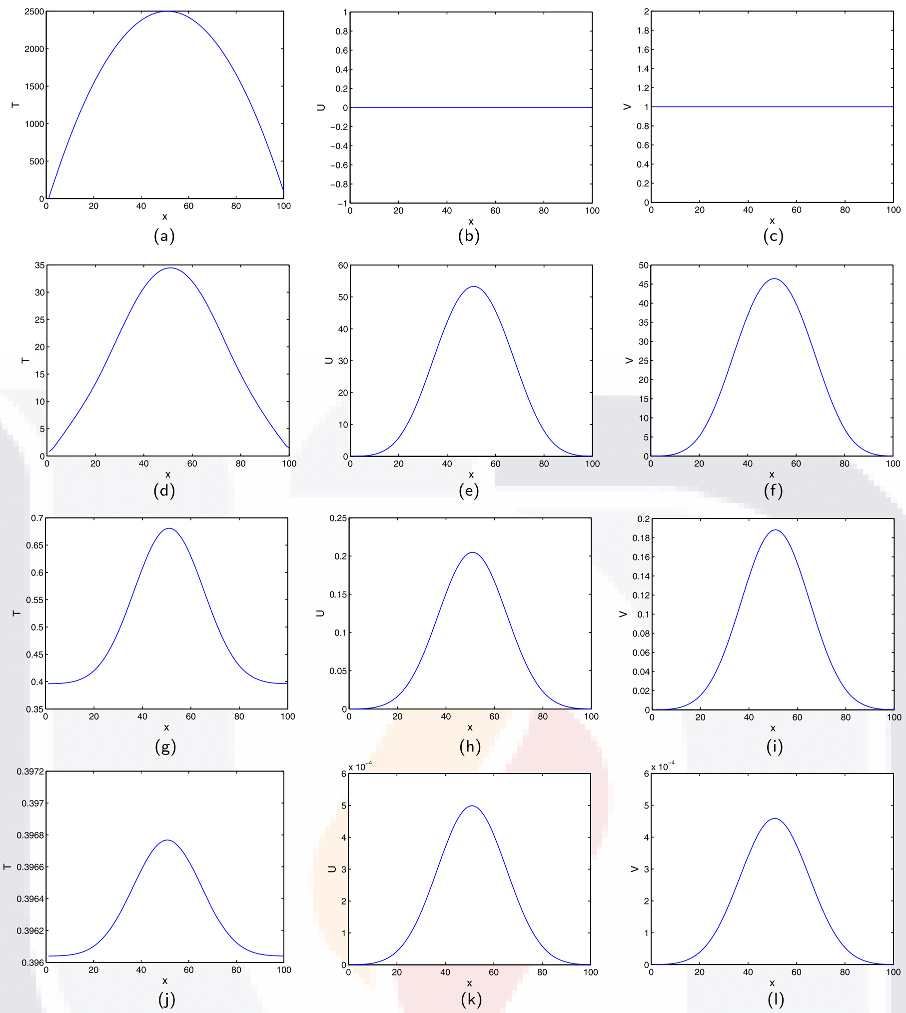

Figure 2 Snapshots of the approximate solutions T, U, and V of (1) for each row at the time $t = 0$, $t = 1$, $t = 3$, and $t = 5$. The parameters employed are $\lambda = 0.1$, $\beta = 2$, $d = 5.05$, $\kappa = 0.03$, $\delta = 0.016$, $\gamma = 3.0$, $c = 20.4$, and $N = 1000$. We let $\phi_T(x)$, $\phi_U(x)$, and $\phi_V(x)$ be as in Example 10. The approximations were calculated using our implementation of (76) in the Appendix, with $\tau = 0.00001$ and $h = 1$

of the normalized solutions T, U, and V at the times $t = 0$, $t = 1$, $t = 3$, and $t = 5$. Once again, the results show that the numerical solutions are positive and bounded.

Before closing this section, we would like to point out the biological meaningfulness of the figures obtained in the previous examples. To start with, graphs (a), (d), (g), and (j) of Fig. 1 represent the evolution with respect to the time of the quantity of the uninfected $CD4^+$T cells. Biologically, the quantity of these cells tends to decrease since there is a significant interaction of the HIV-1 infection with the $CD4^+$T cells, resulting in an increment of them. The respective increments of the infected $CD4^+$T cells with respect to the time are shown in graphs (b), (e), (h), and (k). Moreover, the quantity of the infected $CD4^+$T cells could decrease since an infected cell could die or return to being an uninfected cell. Obviously, this phenomenon is biologically possible. In turn, graphs (c), (f), (i), and (l) represent the evolution of the HIV-1 infection. From these graphs, it is easy to see that the infection is decreasing with respect to the time due to the presence of an active death rate. The interpretation of the graphs in Fig. 2 is analogous.

5 Conclusions

In this manuscript, we numerically studied a coupled model consisting of three diffusive nonlinear partial differential equations. The system under investigation is a biological model which describes the interaction of the HIV-1 infection with the $CD4^{+}T$ cells. One of the equations of the model describes the rate of change of the density of the uninfected $CD4^{+}T$ cells, the second describes the rate of change of the infected $CD4^{+}T$ cells, and the third governs the rate of change of the free HIV-1 infection. The differential system was discretized using finite differences to estimate the analytical solutions. The technique that we used in this work is an exponential type that maintains the most important characteristics of the solutions of the continuous model. More concretely, the method was motivated by the well-known family of Bhattacharya exponential-type schemes [22–24]. Bhattacharya's discretizations have been employed to derive computational techniques to solve various nonlinear partial differential equations [25–28]. As it is well known, the main advantage of this family of models is its computational efficiency.

The scheme presented in this work was analyzed to study its most important properties. The most important structural features proved in this work were related to the unique solvability of the discrete model. We also established that the scheme is able to preserve the nonnegativity and the boundedness of the estimations. These properties are highly relevant in light that the functions under investigation represent densities which are positive and bounded. From the numerical point of view, we proved the consistency of the scheme. Moreover, the method is stable, and it converges to the exact solutions with first order in the temporal variable and second order in the spatial. Finally, we provided some computational simulations to illustrate the capability of the scheme to preserve the positivity and the boundedness of the numerical solutions. A Matlab implementation of the method is provided in the Appendix for reproducibility purposes. It is worth pointing out that a study of the mathematical model (1) in two dimensions can be easily performed by extending the theoretical results of this work. Also, an implementation of our scheme in two dimensions is also easily feasible.

Before we close this work, there are various important comments that require to be thoroughly addressed. To start with, it is important to point out that there are some works in the literature where fractional-type models like (1) without diffusion have been investigated [9, 14]. Naturally, one would wonder which are the effects of considering a fractional diffusion in such HIV-1 systems. At this point, it is important to mention that one of the authors of the present manuscript has devoted part of his efforts to develop numerical methods for Riesz space-fractional partial differential equations [29, 30]. In that context, the differentiation order of the diffusion terms affect the speed of propagation of the spread of effects into the medium. Of course, it would be interesting to propose and analyze numerical models for fractional forms of the system under current investigation. However, the meaningfulness of the use of fractional derivatives in the realistic investigation of HIV-1 may be still questionable. Indeed, not many medical journals employ fractional operators to model the propagation of HIV-1, though the problem is mathematically interesting and challenging.

Appendix: Matlab code

The following is a Matlab implementation of (8). This code was used to approximate the solutions of problem (76) with different initial conditions. Some variations in the coding were performed to obtain the computer results in this manuscript. A commented version of this code and a two-dimensional extension of this algorithm are available from the authors upon request.

```
function [T,U,V,x]=vihFDB

  N=1000;
  delta=0.016;
  kappa=0.03;
  gamma=3.0;
  c=20.4;
  beta=2;
  d=5.05;

  a=0;
  b=100;
  K=5;
  h=1;
  tau=0.00001;
  lambda=0.1;

  x=a:h:b;
  M=length(x);

  T=-1*x(1,1:M-1).^2 + 100*x(1,1:M-1);
  U=zeros(1,M-1);
  V=ones(1,M-1);

  aT=(1/h^2)*[T(1,2:M-1),T(1,M-1)];
  eT=(1/h^2)*[T(1,1),T(1,1:M-2)];

  aU=(1/h^2)*[U(1,2:M-1),U(1,M-1)];
  eU=(1/h^2)*[U(1,1),U(1,1:M-2)];

  aV=(1/h^2)*[V(1,2:M-1),V(1,M-1)];
  eV=(1/h^2)*[V(1,1),V(1,1:M-2)];

  I=floor(K/tau);

  for k=1:I
    WT=beta-(kappa*V+d+(2/h^2)).*T+gamma*U+aT+eT;
    T=(T+lambda).*exp((tau*WT)./(T+lambda))-lambda;

    WU=kappa*(V.*T)-(gamma+delta+(2/h^2))*U+aU+eU;
    U=(U+lambda).*exp((tau*WU)./(U+lambda))-lambda;

    WV=N*delta*U-(c+(2/h^2))*V+aV+eV;
    V=(V+lambda).*exp((tau*WV)./(V+lambda))-lambda;

    aT=(1/h^2)*[T(1,2:M-1),T(1,M-1)];
    eT=(1/h^2)*[T(1,1),T(1,1:M-2)];

    aU=(1/h^2)*[U(1,2:M-1),U(1,M-1)];
    eU=(1/h^2)*[U(1,1),U(1,1:M-2)];
```

```
    aV=(1/h^2)*[V(1,2:M-1),V(1,M-1)];
    eV=(1/h^2)*[V(1,1),V(1,1:M-2)];
  end
end
```

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Competing interests
The authors declare that they have no competing interests.

Authors' contributions
Conceptualization, JAP and JEMD; methodology, JAP; software, JAP and JEMD; validation, JAP and JEMD; formal analysis, JAP and JEMD; investigation, JAP and JEMD; resources, JAP and JEMD; data curation, JAP and JEMD; writing–original draft preparation, JAP and JEMD; writing–review and editing, JAP and JEMD; visualization, JAP; supervision, JEMD; project administration, JEMD; funding acquisition, JEMD. All authors read and approved the final manuscript.

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4. Conclusions and discussions

In chapter 1, we investigated numerically a system of two parabolic partial differential equations with coupled nonlinear reaction terms in generalized forms. The system considers the presence of anomalous diffusion in multiple spatial dimensions along with suitable initial data. The model generalizes various particular systems from the physical sciences, including the diffusive systems which describe the interaction between populations of predators and preys with Michaelis–Menten-type reaction. The system is discretized following a finite-difference approach, and two schemes are proposed to approximate the solutions. The two numerical models are analyzed for structural and numerical properties.

As the main structural results, we establish the existence and uniqueness of the numerical solutions. Moreover, we prove that the schemes are both capable of preserving the positivity and boundedness of approximations. This is in perfect agreement with the fact that the relevant solutions of normalized population models are positive and bounded. Numerically, we prove rigorously that the schemes are consistent, stable and convergent. Some simulations are provided in this work to illustrate the performance of the schemes. In particular, we show the capability of one of the schemes to be applied on the investigation of Turing patterns in anomalously diffusive systems describing predator-prey interactions. To that end, a fast computational implementation in Fortran of one of the schemes is employed.

In chapter 2, we considered a general system of partial differential equations with nonlinear coupled reaction terms. The system considered hyperbolic terms and constant damping coefficients along with fractional diffusion of the Riesz type. The system considered a finite though arbitrary number of spatial coordinates. Also, a finite and arbitrary number of equations was considered herein, making our model sufficiently general to be able to describe various problems from the physical sciences. A structure-preserving finite-difference discretization based on the use of fractional-order centered differences was presented here to solve the continuous model. The scheme is a three-step model, which may be nonlinear depending on the expressions of the reaction terms. Using Brouwer's fixed-point theorem, we established rigorously the existence of solutions of the discrete model. Moreover, we provided sufficient conditions to guarantee the preservation of the positivity and the boundedness of the scheme. In that sense, our numerical technique is a structure-preserving technique which is numerically efficient. Indeed, we proved mathematically that the methodology proposed in this work is consistent of second order in both space and time. Using a discrete form of the energy method, we established the stability of the discrete model along with the second-order convergence in space and time. As a corollary of the stability of our scheme, the uniqueness of the solutions of the method is a straightforward corollary. Some illustrative simulations were provided in order to show the capability of the scheme to reproduce Turing patterns in a hyperbolic reaction-diffusion system. The simulations were obtained through a computer implementation of the discrete model, and they showed that the scheme is capable of preserving both the positivity and the boundedness of approximations.

In chapter 3, we numerically studied a coupled model consisting of three diffusive nonlinear partial differential equations. The system under investigation is a biological model which describes the interaction of the HIV-1 infection with the CD4 T cells. One of the equations of the model describes the rate of change of the density of the uninfected CD4 T cells, the second describes the rate of change of the infected CD4 T cells, and the third governs the rate of change of the free HIV-1 infection. The differential system was discretized using finite differences to estimate the analytical solutions. The technique that we used in this work is an exponential type that maintains the most important char acteristics of the solutions of the continuous model. More concretely, the method was motivated by the well-known family of Bhattacharya exponential-type schemes. Bhattacharya's discretizations have been employed to derive computational techniques to solve various nonlinear partial differential equation. As it is well known, the main advantage of this family of models is its computational efficiency. he scheme presented in this work was analyzed to study its most important properties. The most important structural features proved in this work were related to the unique solvability of the discrete model. We also established that the scheme is able to preserve the nonnegativity and the boundedness of the estimations. These properties are highly relevant in light that the functions under investigation represent densities which are positive and bounded. From the numerical point of view, we proved the consistency of the scheme. Moreover, the method is stable, and it converges to the exact solutions with first order in the temporal variable and second order in the spatial. Finally, we provided some computational simulations to illustrate the capability of the scheme to preserve the positivity and the boundedness of the numerical solutions.

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