CENTRO DE CIENCIAS BÁSICAS

DEPARTAMENTO DE MATEMÁTICAS Y FÍSICA

TESIS

ANALYSIS AND SIMULATION OF PATTERN FORMATION IN FRACTIONAL HYPERBOLIC SYSTEMS

PRESENTA

José Rivera López Rayón

PARA OPTAR POR EL GRADO DE MAESTRO EN CIENCIAS EN MATEMÁTICAS APLICADAS

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Aguascalientes, Ags., 6 de enero de 2020

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

TITULO: ANALYSIS AND SIMULATION OF PATTERN FORMATION IN FRACTIONAL HYPERBOLIC SYSTEMS

IMPACTO SOCIAL (señalar el impacto logrado): Utilizando herramientas matemáticas, numéricas y computacionales se determinaron las condiciones para la aparición de patrones de Turing en sistemas químicos realistas.

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José Rivera López Rayón

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Abstract

In this thesis, firstly we investigate a hyperbolic partial differential equation that generalizes the classical wave equation. The model considers a spatial Laplatian of fractional order in terms of Riesz fractional derivatives, and a generalized potential function. To approximate the solution of this model we propose a finite difference method with second-order consistency based on fractional centered differences. This numerical approximation, besides of being stable and convergent, has the property of conserving or dissipating the system's energy under the same parametric and boundary conditions as the continuous model. In the second part, we study a generalized form of a two-dimensional coupled hyperbolic system that describes an activator-inhibitor chemical reaction that produces stationary spatial structures known as Turing patterns. The reaction terms are polynomial type and the diffusive terms are fractional Riesz Laplacians with differentiation orders in (0,1) (subdiffusion) and (1,2] (superdiffusion). A finite-difference methodology based on the use of fractional centered differences was designed to approximate the solutions of the problem. We prove the existence and the uniqueness of the solutions of the numerical method and establish its main numerical properties, namely, quadratic consistency, stability and quadratic convergence. Numerical simulations show the appearance of Turing patterns under subdiffusive conditions, and not only under the scenario previously reported in literature of superdiffusive conditions.

Resumen

En esta tesis, en primer lugar estudiamos una ecuación diferencial parcial hiperbólica fraccionaria que generaliza la ecuación de onda clásica. El modelo considera un laplaciano espacial en términos de la derivada fraccionaria de Riesz, y una función de potencial generalizada. Para aproximar la solución de este modelo proponemos un método de diferencias finitas con orden de consistencia cuadrático, el cual incorpora diferencias centradas fraccionarias. Esta aproximación numérica, además de ser estable y convergente, tiene la propiedad de conservar o disipar la energía del sistema bajo las mismas condiciones paramétricas y de frontera que el modelo continuo. En la segunda parte, estudiamos una forma generalizada de un sistema hiperbólico bidimensional que describe una reacción química de tipo activador-inhibidor que produce patrones espaciales estacionarios conocidos como patrones de Turing. Los términos de reacción son de tipo polinomial, en tanto que los términos de difusión son laplacianos fraccionarios de Riesz con órdenes de diferenciación en (0,1) (subdifusión) y (1,2] (superdifusión). Para aproximar las soluciones del problema se diseñó una metodología de diferencias finitas basada en el uso de diferencias centradas fraccionarias. Demostramos la existencia y unicidad de las soluciones del método numérico y establecemos sus principales propiedades numéricas, a saber, consistencia cuadrática, estabilidad y convergencia cuadrática. Las simulaciones numéricas del método muestran, tal como lo reportan otros estudios, la aparición de patrones de Turing en escenarios de superdifusión. Adicionalmente, mostramos que los patrones de Turing también se presentan bajo condiciones de subdifusión.

Introduction

Aims and scope

The design of numerical methods that preserve the discrete energy of conservative systems governed by partial differential equations has been an important area of research in computational physics [20, 127]. Many different approaches have been employed in order to provide numerical techniques that preserve the total energy of discrete models, including finite differences [141], mimetic finite differences [71], finite elements [47], Galerkin methods [33], symplectic techniques [130], G-symplectic schemes [26] and finite pointset methods [73] among other approaches. Historically, the development of numerical techniques that preserve physical properties of the solutions of systems of partial differential equations was popularized by D. Furihata and coworkers at the turn of the 21st century [43, 44]. Many reports on the design of numerical techniques that preserve physical or mathematical invariants of systems of partial differential equations were proposed afterwards [19], including manuscripts on methods that preserve the mass [55] and the momentum [117] of a system. Of course, many physical applications have been proposed using those techniques.

The design of techniques to approximate the solution of physical systems has been largely enriched with the study of partial differential equations of fractional orders. Indeed, fractional calculus has found interesting applications in many fields of the natural sciences and engineering, including the theory of viscoelasticity [60], the theory of thermoelasticity [100], financial problems under a continuous time frame [109], self-similar protein dynamics [49] and quantum mechanics [90]. Distributed-order fractional diffusion-wave equations are used in groundwater flow modelling to and from wells [115, 98]. A vast amount of nonequivalent approaches have been followed, and new criteria of fractional differentiation have been proposed constantly in the last decades. However, the problem in those cases is the common lack of a physically meaningful formulation of the Euler–Lagrange formality for fractional variational systems [1]. As expected, this has been a major problem in the design of energy-preserving method for fractional partial differential equations.

In spite of this shortcoming, many of the partial differential equations from mathematical physics have been extended to the fractional scenario. Physically, problems that only considered local contributions to the dynamics of discrete or continuous systems have been extended to account for global effects. In such way, various classical models that were traditionally described by partial differential equations have been formulated using derivatives of fractional order under different approaches [108, 91, 122]. Among the models that have been extended to the fractional scenario are the classical nonlinear wave equations [103, 5]. Here, it is important to point out that the Riesz definition of spatial derivatives of fractional order has been extensively employed in order to account physically for anomalous diffusion [51], and to provide pertinent conservation laws and Hamiltonian-like equations [125]. In view of these remarks, a natural question that arises immediately is whether it is feasible to propose finite-difference discretizations of nonlinear hyperbolic equations with Riesz space-fractional derivatives, in such way that known conservation laws are likewise conserved in the discrete domain.

The purpose of this thesis is, in the first part, to approximate a nonlinear dissipative wave equation with Riesz space-fractional derivatives using a finite-difference discretization based on fractional centered differences. We will establish the capability of the finite-difference scheme to preserve the dissipation or the conservation of energy of the discrete system. Furthermore, we will show that our method is a consistent

technique and we will establish the stability and the convergence properties of our scheme. In the second part, we investigate numerically a generalized two-dimensional hyperbolic system with anomalous diffusion that describes the interaction between an activator and an inhibitor in chemical reactions. Again, we provide a discretization using fractional centered differences. The use of a fixed-point theorem as well as some properties of fractional discrete operators will allow us to prove the existence (and uniqueness) of solutions of the numerical method. Employing Taylor series, we establish the method's second order of consistency. Additionally, the discrete energy method will be employed to prove the stability and convergence properties. Some computational simulations are carried out in order to validate our code and to identify conditions for the presence of Turing patterns.

Summary

This thesis is sectioned as follows.

- Chapter 1 provides a list of important second-order partial differential equations that constitute particular cases of the equation under study. We state the general form of our problem, describe the most important applications that it models, and provide analytical methods to compute solution and, particularly, soliton-like solutions to several particular cases. We close this chapter stating some important definitions and results from numerical analysis that we use in this thesis without reference.

- Chapter 2 deals with a nonlinear dissipative wave equation with Riesz space-fractional derivatives. We present an energy functional proposed in the literature and show that the initial-boundary-value problem is conservative or dissipative under suitable analytic conditions. The concept of fractional centered differences is recalled and a numerical method to approximate the equation's solution is proposed. The most important physical properties of the method are analyzed, particularly the capability of preserving the dissipation or conservation of energy of the discrete system. Next, the most important numerical properties of our technique (consistency, stability and convergence) are stablished. Some computational simulations are presented in the final section of this chapter.

- Chapter 3 presents a numerical method to approximate a two-dimensional hyperbolic system describing the interactions of and activator-inhibitor chemical reaction subject to fractional diffusion. Initial conditions are imposed on a closed and bounded rectangle and a finite difference method employing fractional centered differences is proposed to approximate the solutions of our generalized model. We establish the solvability of our numerical technique, and show that the method is a quadratically consistent, stable and quadratically convergent. Computer simulations are provided, exhibiting the presence of Turing patterns under suitable parameter conditions.

1. Preliminaries

The nonlinear Klein-Gordon equation is one of the most important and simplest nonlinear differential equations that appear in relativistic quantum mechanics. As a second-order partial differential equation, the Klein-Gordon equation generalizes several other important problems in various branches of physics, chemistry and mathematical biology that range from the classical diffusion equation to the stochastic Fisher-KPP equation, from the classical wave equation to the Schrödinger and the telegrapher's equations. The present chapter is devoted to introduce and evidence the importance of the differential equation under study in this thesis. We also present some important definitions and results of numerical analysis that will be used without reference in further chapters.

1.1 Basic definitions

By a **domain** we understand a closed connected subset of $\mathbb{R}^n$. A function u defined in a domain D is said to be have **compact support** if it is zero outside a compact subset of D. A function u defined on a domain D is called **smooth** in D if it has continuous partial derivatives of all orders in D. The function u is called **small at infinity** if for every $\bar{x}_0$ in the boundary of D,

$$\lim_{\substack{\bar{x} \to \bar{x}_0 \\ \bar{x} \in D}} u(\bar{x}) = 0.$$

Let a, b, c, d and e be real numbers with at least one of a, b or c not equal to zero. A second-order partial differential equation in the variables x and y with constant coefficients is an equation of the form

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} = F(x, y), \tag{1.1}$$

where u is a function of (x, y) usually assumed to be defined and of compact support in some domain D, that has continuous partial derivatives up to the second order in D. The number $b^2 - 4ac$ is called the **discriminant** of Equation (1.1) and yields a criterion to classify second-order partial differential equations:

- If $b^2 - 4ac > 0$ then Equation (1.1) is called a **hyperbolic** equation. As an example of this type of equation we have the classical one-dimensional **wave equation**

  $$\frac{\partial^2 u}{\partial x^2} = \frac{1}{\nu^2}\frac{\partial^2 u}{\partial t^2}.$$

  It describes the vertical disturbance of a wave with phase velocity ν as it travels on the horizontal direction. The wave equation applies to a stretched string or a plane electromagnetic wave. Given initial and boundary conditions the wave equation can be solved exactly by using a Fourier transform method or via separation of variables.

- If $b^2 - 4ac = 0$ then Equation (1.1) is called a **parabolic** equation. An example of parabolic equation is the one-dimensional **diffusion equation** (also called **heat equation**)

  $$\frac{\partial u}{\partial t} = \kappa\frac{\partial^2 u}{\partial x^2}.$$

This equation commonly arises in problems of heat conductivity. In those situations κ represents thermal diffusivity and u represents temperature. If initial and boundary conditions are given, the diffusion equation can be solved analytically by separation of variables.

- If $b^2 - 4ac < 0$ then Equation (1.1) is called an **elliptic** equation. **Laplace's equation**

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

is an example of an elliptic equation. It is satisfied by the potential of any distribution of matter which attracts according to the Newtonian Law. A solution to Laplace's equation is uniquely determined if the value of the function or the normal derivative of the function is specified on all boundaries.

We must remark that the wave equation, the heat equation and Laplace's equation have generalizations that model the corresponding physical phenomena in three dimensions. For example, the **wave equation** in three space variables reads

$$\nabla^2 u = \frac{1}{\nu^2}\frac{\partial^2 u}{\partial t^2},$$

where u is a scalar function that depends on the space coordinate (x, y, z) and time t. The symbol ∇^2 denotes the **Laplacian** differential operator, which is the divergence of the gradient of a scalar function. With this notation the three-dimensional **diffusion equation** is described by the equation

$$\frac{\partial u}{\partial t} = \frac{1}{\kappa}\nabla^2 u,$$

and the three-dimensional **Laplace's equation** by

$$\nabla^2 u = 0.$$

Let V and ρ be scalar functions depending only on space. An important variation of the three-dimensional Laplace's equation occurs in classical electromagnetic theory when relating the electric potential V of a distribution and its charge density ρ. The relation between V and ρ is described by the equation $\epsilon_0 \nabla^2 V = \rho$, which is called **Poisson's equation**. More generally, every equation of the form

$$\nabla^2 u = F(x, y, z, t),$$

where u is a scalar function depending on x, y, z and t, is called a Poisson equation. Another useful classification of second-order partial differential equations with constant coefficients is in terms of a property called *linearity*. Differential equation (1.1) is called **linear** if for arbitrary real constants k_1, k_2 and solutions u_1, u_2 of (1.1), $k_1 u_1 + k_2 u_2$ is also a solution of (1.1).

Finally, if the variable time is one of the independent variables of the scalar function u then the term $k\partial u/\partial t$ in the differential equation modeling u is called the **external damping term** and the constant k is called the **external damping coefficient**. The differential equation is said to be **damped** if k is not equal to zero, otherwise it is called **undamped**.

1.2 Important partial differential equations

Many other three-dimensional generalizations of the wave equation, the diffusion equation and Laplace's equation happen to appear in mathematical physics and biology. For example, the manipulation of Maxwell's equations to obtain propagating waves gives rise to the so called **Helmholtz equation** [146], whose general form is

$$\nabla^2 u + k^2 u = 0,$$

where k is a real constant and u is a scalar function in the variables x, y, z, t. Obviously, Helmholtz equation is a linear second-order partial differential equation that generalizes the three-dimensional wave equation.

Another physical example appears in the field of non-relativistic quantum mechanics: Let $\hbar$ denote Planck's original constant divided by 2π. The wave function associated to a particle of mass m with

potential scalar function V is a scalar function u that depends on the position vector (x, y, z) of the particle and the time t, given by the differential equation

$$i\hbar\frac{\partial u}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 u + Vu.$$

This differential equation is called **Schrödinger's equation**. In this equation the scalar function u may be complex, but the square of its modulus is a real scalar function that represents the probability density function associated with the location of the particle at any time. It is worth noticing that Schrödinger's equation provides a mathematical generalization of the three-dimensional diffusion equation. Observe that because the scalar function V does not need to be constant, Schrödinger's equation is a linear partial differential equation with not necessarily constant coefficients.

The relativistic counterpart of Schrödinger's equation is the Klein-Gordon equation. By the **linear Klein-Gordon equation** we understand the linear second-order partial differential equation

$$\nabla^2 u = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} + m^2 u,$$

where m is a real constant and u is a scalar function of position and time. This is the equation for a relativistic quantum-mechanical scalar (spin-zero) particle of mass m. The exact solution of this equation in the form of a traveling wave is given in [99]. An important nonlinear variation of this equation that often appears in the study of the collisional properties of **solitons** [97, 116], that is solitary waves, and a number of other physical applications [8, 48, 13] is the **sine-Gordon equation**

$$\nabla^2 u = \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} + m^2 \sin u.$$

Several nonlinear variations of the Klein-Gordon equation appear in many branches of physics, chemistry and other sciences. The **Landau-Ginzburg equation** is one of those equations. Studied by Lev Landau and Vitaly Ginzburg in 1950 while studying the theory of superconductivity, this equation is used to study simple periodic oscillations and the change of their amplitude and frequency with respect to initial excitations in problems that arise in oscillating chemical reactions and atomic physics. In dimensionless form, the three-dimensional Landau-Ginzburg equation is given by

$$\frac{\partial^2 u}{\partial t^2} - \nabla^2 u - m^2 u + G'(u) = 0$$

In mathematical biology, consider a population distributed in a linear habitat with uniform density. If at any point of the habitat a mutation advantageous to survival occurs then the mutant gene increases at the expense of the allelomorphs previously occupying the same locus. Mathematically, let u be the frequency of the mutant gene and let m be a constant representing intensity of selection in favor of the mutant gene. Then u must satisfy **Fisher's equation** (also called the **Fisher-KPP equation**)

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} + F(u),$$

where k is a diffusion coefficient and u depends on the position x in the linear habitat and time t given in generations. This parabolic equation was simultaneously and independently investigated by Fisher [37] and Kolmogoroff *et al.* [61], using $F(u) = mu(1-u)$. It is used also in describing the process of epidermal wound healing [111]. Other applications appear in the theory of superconducting electrodynamics [129] and in the study of excitons [102]. Fisher's equation is a nonlinear equation that obviously generalizes the three-dimensional diffusion model if we rewrite Fisher's equation as

$$\frac{\partial u}{\partial t} = k\nabla^2 u + F(u).$$

The **stochastic Fisher-KPP equation** is the one-dimensional Fisher equation with $F(u) = mu(1-u)+\gamma\sqrt{u(1-u)}\eta(x,t)$, where $0 \leq u \leq 1$, γ is a real constant, and $\eta(x,t)$ is a *Gaussian white noise process* in space and time with mean equal to zero [29]. To fix ideas, we may think of a **noise** as a random signal of known statistical properties of amplitude, distribution, and spectral density. A noise is a **white noise**

in space and time if it is uncorrelated in these two variables, and it is **Gaussian** if its probability density function over a given frequency band is normal. The stochastic Fisher-KPP equation is a stochastic partial differential equation that describes random walk processes that have applications in hydrodynamics and economics.

Second-order partial differential equations describing diffusion or conduction happen to appear in the area of thermodynamics [85]. Heat conduction is understood as the transfer of heat from warm areas to cooler ones, and effectively occurs by diffusion. Under the assumption of a macroscopic continuum formulation, the **Fourier equation** [39] for the heat flux $\bar{q}$ in a medium of density ρ, mass heat capacity C_P, and temperature function u, is

$$\bar{q} = -k\nabla u,$$

where both $\bar{q}$ and u depend on the three spatial coordinates and time, $k = \rho\kappa C_P$ is the thermal conductivity of the medium, and κ is the thermal diffusivity term of the classical diffusion equation.

The previously mentioned Fourier heat conduction equation is diffusive and does not account for the temperature propagation speed in transient situations. Because of certain issues argued and identified earlier, attempts to account for a finite speed of heat propagation have evolved over the years. The **Maxwell-Cattaneo model** [17], which is based on the notion of relaxing the heat flux, is given as

$$\tau\frac{\partial\bar{q}}{\partial t} = -\bar{q} - k\nabla u,$$

where τ is the relaxation time. Assuming that there are no heat sources and that k is constant, the one-dimensional version of the Maxwell-Cattaneo equation together with the energy equation

$$\rho C_P\frac{\partial u}{\partial t} + \frac{\partial q}{\partial x} = 0,$$

yield the hyperbolic equation

$$\tau\rho C_P\frac{\partial^2 u}{\partial t^2} - k\frac{\partial^2 u}{\partial x^2} + \rho C_P\frac{\partial u}{\partial t} = 0.$$

Obviously, it can be generalized to the three-dimensional case as

$$\frac{\partial^2 u}{\partial t^2} - \frac{k}{\tau\rho C_P}\nabla^2 u + \frac{1}{\tau}\frac{\partial u}{\partial t} = 0.$$

The **telegraph equation** is a hyperbolic equation that describes heat or mass transport. It models phenomena that are mixtures between diffusion and wave propagation. In this model a small section of a telegraph wire is treated to study the pulse of voltage moving along the wire. It was studied in 1876 by Heaviside in his research on coaxial marine telegraph cables [70]. The telegraph equation is the linear second-order partial differential equation

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{\nu^2}\frac{\partial^2 u}{\partial t^2} - \gamma\frac{\partial u}{\partial t} - b^2 u = 0,$$

where ν is positive, and γ and b are nonnegative constants. The one-dimensional wave equation is just a particular case of the telegraph equation with γ and b both equal to zero. The generalization of the telegraph equation to three dimensions is

$$\nabla^2 u - \frac{1}{\nu^2}\frac{\partial^2 u}{\partial t^2} - \gamma\frac{\partial u}{\partial t} - b^2 u = 0.$$

1.3 Modified Klein-Gordon equations

The objective of this section is to study a general form of the Klein-Gordon equation that embraces the partial differential equations described in the previous section and, at the same time, takes into account a third-order term proportional to the Laplacian of the partial derivative of u in time, which physically represents the **internal damping term**. More precisely, let u be a function of the spatial variables X, Y, Z, and the time variable T. The nonlinear partial differential equation with constant coefficients that we wish to study in this thesis is

$$a\frac{\partial^2 u}{\partial T^2} - b\nabla^2 u - c\frac{\partial}{\partial T}\left(\nabla^2 u\right) + d\frac{\partial u}{\partial T} + m^2 u + G'(u) = 0,$$

Let $x = X/\sqrt{b}$, $y = Y/\sqrt{b}$, $z = Z/\sqrt{b}$, and $t = T/\sqrt{a}$ for a and b positive numbers. Let $\beta = c/(b\sqrt{a})$ and $\gamma = d/\sqrt{a}$. Our problem can be stated in dimensionless form as

$$\frac{\partial^2 u}{\partial t^2} - \nabla^2 u - \beta \frac{\partial}{\partial t}\left(\nabla^2 u\right) + \gamma \frac{\partial u}{\partial t} + m^2 u + G'(u) = 0,$$
$$\text{subject to : } \begin{cases} u(\bar{x}, 0) = \phi(\bar{x}), & \bar{x} \in D, \\ \dfrac{\partial u}{\partial t}(\bar{x}, 0) = \psi(\bar{x}), & \bar{x} \in D. \end{cases} \tag{1.2}$$

This initial-value problem will be referred to as the **modified nonlinear Klein-Gordon equation** or the **dissipative nonlinear Klein-Gordon equation**, and its numerical study for the particular choice $G'(u) = u^p$, for $p > 1$ an odd number, is the topic of this section. We identify the term containing the coefficient β as the internal damping term, while the term containing γ is easily identified as the external damping term. Needless to say that the differential equation in (1.2) generalizes the equations listed in Section 1.2 either by choosing suitable coefficients or by suppressing terms; the classical Klein-Gordon equation, for instance, can be obtained by setting β and γ both equal to zero and G' identically zero. It is worthwhile mentioning that the undamped nonlinear Klein-Gordon equation with $G'(u) = u^3$ is called the **quasilinear Klein-Gordon equation**, and it also has physical applications [92].

The following is the major theoretic result we will use in our investigation. It is valid only for certain classical one-dimensional nonlinear Klein-Gordon equations. Here $M(t)$ represents the amplitude of a solution of (1.2) at time t, that is

$$M(t) = \max_x |u(x,t)|.$$

Theorem 1.3.1. *Let β and γ be both equal to zero, and let $G'(u) = |u|^{p-1}u$. Suppose that ϕ and ψ are smooth and small at infinity. Then*

(1) *If $p < 5$, a unique smooth solution of* (1.2) *exists with amplitude bounded at all time* [57].

(2) *If $p \geq 5$, a weak solution exists for all time* [110].

(3) *For $p > 8/3$ and for solutions of bounded amplitude, there is a scattering theory; in particular, they decay uniformly as fast as $M(t) \leq c(1 + |t|)^{-3/2}$* [88]. □

Josephson transmission lines

As we stated in the introductory chapter, initial-value problem (1.2) has applications in several physical problems. In the remainder of this section we will describe some of them.

A **Josephson junction** is a type of electronic circuit capable of switching at very high speeds when operated at temperatures approaching absolute zero. Named for the British physicist who designed it, a Josephson junction exploits the phenomenon of superconductivity, that is the ability of certain materials to conduct electric current with practically zero resistance. Josephson junctions are used in certain specialized instruments such as highly-sensitive microwave detectors, magnetometers, and quantum interference devices.

A Josephson junction is made up of two superconductors, separated by a nonsuperconducting layer so thin that electrons can cross through the insulating barrier. The flow of current between the superconductors in the absence of an applied voltage is called a **Josephson current**, and the movement of electrons across the barrier is known as **Josephson tunneling**. Two or more junctions joined by superconducting paths form what is called a **Josephson interferometer.**

While researching superconductivity, Josephson studied the properties of a junction between two superconductors [58]. Following up on earlier works by Leo Esaki and Ivar Giaever, he demonstrated that in a situation when there is electron flow between two superconductors through an insulating layer (in the absence of an applied voltage), and a voltage is applied, the current stops flowing and oscillates at a high frequency. This phenomenon is called the **Josephson effect**, and it is influenced by magnetic fields in the vicinity, a capacity that enables the Josephson junction to be used in devices that measure extremely weak magnetic fields, such as superconducting quantum interference devices. For their efforts, Josephson, Esaki, and Giaever shared the Nobel Prize for Physics in 1973.

It is worthwhile mentioning that the theory of low temperature conductivity tells us that a superconductor is a system where a fraction of the conduction electrons form pairs called **Cooper pairs**. In these

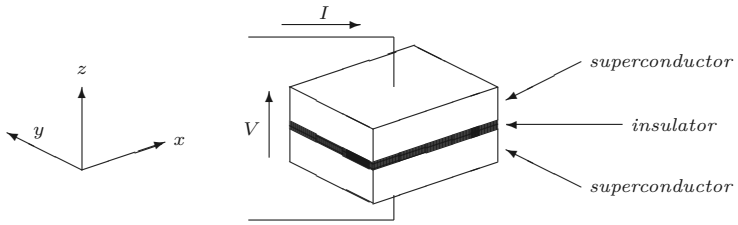

Figure 1.1: Schematic representation of a small Josephson junction.

pairs the two electrons have opposite momentum and spin. These pairs are able to condense in the same quantum state so that the superconductor can be described by a single macroscopic wave function

$$\Psi = \sqrt{\rho} e^{i\phi}.$$

Here ρ represents the pair density and ϕ is the quantum phase common to all pairs. A **small Josephson junction** consists of two small layers of superconducting metal separated by a thin dielectric barrier layer, which is small enough to permit tunneling of Cooper pairs (equivalently, coupling of the wave functions of the two superconductors).

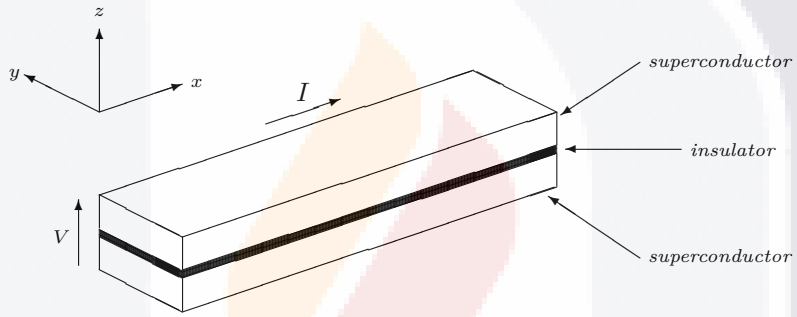

Figure 1.2: Schematic representation of a long Josephson junction.

A **long Josephson junction** consists of two identical superconducting long strips separated by a thin dielectric layer. This long tunneling junction can be regarded as a transmission line as far its electromagnetic behavior is concerned [8]. However, in dealing with real transmission lines for the long Josephson junction one must take into account losses, bias, and junction irregularities which influence motion [104]. When we account for all of these effects, we obtain the third-order partial differential equation

$$\frac{\partial^2 \phi}{\partial x^2} - \frac{\partial^2 \phi}{\partial t^2} - \alpha \frac{\partial \phi}{\partial t} + \beta \frac{\partial^3 \phi}{\partial x^2 \partial t} = \sin \phi - \gamma,$$

where α, β and γ are constants.

The statistical mechanics of kinks

The statistical mechanics of **kinks** (that is, exact solitary waves) of nonlinear coherent structures has been studied by two approaches. In the first approach one assumes that the kinks may be treated as weakly interacting elementary excitations. Provided the kink density is low, the canonical partition function can be found by standard methods [83, 64, 25]. Alternatively, it is possible to calculate the partition function to exploit a transfer operator technique. This method was used by Krumhansl and Schrieffer in [64], and it showed that in the low temperature limit the partition function naturally factorizes into two contributions: A tunneling term which they were able to identify with the kink contribution, and the remainder which they identified as linearized phonons (by a **phonon** we mean a quantized mode of vibration occurring in a rigid crystal lattice, such as the atomic lattice of a solid).

The ideas of Krumhansl and Schrieffer were further refined and extended to a wider class of systems [25]. In particular, interactions of kinks with linearized phonons were considered, leading to substantial

corrections of results. Computer simulations based on standard methods [4] made possible to verify results on the equilibrium statistical mechanics of kinks using a dimensionless **Langevin equation** describing the $(1+1)$-dimensional theory:

$$\frac{\partial^2\phi}{\partial t^2} = \frac{\partial^2\phi}{\partial x^2} - \gamma\frac{\partial\phi}{\partial t} - \phi(1-\phi^2) + F(x,t).$$

The wave equation revisited

Initial-value problem (1.2) also describes the mechanical motion of strings for certain physical situations. Consider the one-dimensional motion of a string immersed in a non-Hookean medium. We represent the vertical motion of the string as a function $u(r,t)$ of horizontal position and time, and the nonlinear force of the medium by $G'(u)$. The string is assumed to posses internal damping due to its inner stiffness, which is proportional to u_{rrt}. Finally, we assume that there exists friction between the string and the medium that derives in a force which opposes the motion of the string and is proportional to the vertical velocity of the string. In these circumstances, the motion of our string will be described by (1.2).

1.4 Elementary solutions

In our study we will be often interested in studying soliton solutions. As mentioned before, solitons are solitary waves found in many nonlinear physical phenomena. They were first named by Zabusky and Kruskal in 1965 [143], and first appeared in the solution of the **Korteweg-de Vries equation**

$$\frac{\partial u}{\partial t} + \frac{\partial^3 u}{\partial x^3} - 6u\frac{\partial u}{\partial x} = 0.$$

Later on it was proved that equations such as the nonlinear Schrödinger equation, the nonlinear Klein-Gordon equation and the sine-Gordon equation also posses soliton solutions. Mathematically, **solitons** have been defined [30] as solutions of nonlinear partial differential equations which

(i) represent waves of permanent form and velocity,

(ii) decay or approach a constant at infinity, and

(iii) can interact strongly with other solitons and retain their identity.

Given a differential equation in the variables x and t, an **elementary soliton solution** is a solution of the differential equation u of the form $u(x,t) = \phi(x-vt)$ with the property that the infinite limits $\lim_{x\to-\infty} u(x,t)$ and $\lim_{x\to+\infty} u(x,t)$ are constant with respect to time. In this section we derive the solution of the linear Klein-Gordon equation using Fourier transforms and some elementary soliton solutions for some important nonlinear partial differential equations. Throughout ξ will denote the quantity $x-vt$.

The linear Klein-Gordon equation

First we wish to use Fourier transform to solve an arbitrary initial value-problem involving the linear Klein-Gordon equation and provide a solution in terms of the source function. After that, we will find the traveling wave solutions of this differential equation. Thus, let m be a real constant and the consider the $(1+1)$-dimensional initial-value problem

$$\frac{\partial^2 u}{\partial t^2} - \nabla^2 u + m^2 u = 0,$$

$$\text{subject to : } \begin{cases} u(x,0) = \phi(x), & \bar{x}\in\mathbb{R}, \\ \dfrac{\partial u}{\partial t}(x,0) = \psi(x), & x\in\mathbb{R}. \end{cases}$$

Using Fourier transform, this problem in terms of the source function $S(x,t)$ can be expressed as the initial-value problem

$$\frac{\partial^2 \hat{S}}{\partial t^2} + k^2 \hat{S} + m^2 \hat{S} = 0,$$

$$\text{subject to : } \begin{cases} \hat{S}(k,0) = 0, & -\pi < k < \pi, \\ \dfrac{\partial \hat{S}}{\partial t}(k,0) = 1, & -\pi < k < \pi. \end{cases}$$

For a fixed value of k, the differential equation in the initial-value problem above is ordinary, and its solution is a linear combination of sines and cosines. It can be seen then that the particular solution to this problem is of the form $\hat{S}(k,t) = \sin(\omega t)/\omega$, where $\omega = \sqrt{k^2 + m^2}$. After applying inverse Fourier transform to $\hat{S}$ and simplifying, it is easy to obtain that

$$S(x,t) = \begin{cases} \dfrac{1}{2} J_0\left(m\sqrt{t^2 - x^2}\right), & \text{for } |x| < t, \\ 0, & \text{for } |x| \geq t, \end{cases}$$

Where J_0 is the Bessel function of the first kind of order 0 whose general definition may be found in [53]. Needless to say that the source function S of the linear Klein-Gordon equation converges to the source function corresponding to the classical wave equation when m tends to 0.

We are interested now in computing radially symmetric solutions of the three-dimensional linear Klein-Gordon equation using Fourier transforms. It is easy to verify that the expression $\hat{S}(\bar{k}, t)$ of the Fourier transform of the source function in this case will be the same as that of the (1+1)-dimensional one. Letting r represent the Euclidean norm of $\bar{x}$ in $\mathbb{R}^3$ and computing the inverse Fourier transform of $\hat{S}$ we get

$$\begin{aligned} S(r,t) &= \frac{1}{8\pi^3} \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} \frac{\sin(\omega t)}{\omega}\ k^2 \sin\theta e^{ikr\cos\theta} dk\ d\theta\ d\phi \\ &= \frac{1}{2\pi r^2} \int_0^{\infty} \frac{\sin(t\sqrt{k^2+m^2})}{\sqrt{k^2+m^2}}\ k \sin kr\ dk \\ &= -\frac{1}{4\pi r} \frac{\delta}{\delta r} \int_{-\infty}^{\infty} \frac{\sin(t\sqrt{k^2+m^2})}{\sqrt{k^2+m^2}}\ e^{ikr} dk. \end{aligned}$$

Let H represent the Heaviside function. Computing the above derivative with respect to r and using the identities $J_0 = -J_1$ and $J_0(0) = 1$, we obtain that

$$S(r,t) = \frac{1}{2\pi}\delta(t^2 - r^2) - mH(t^2 - r^2)\frac{J_1(m\sqrt{t^2 - r^2})}{4\pi\sqrt{t^2 - r^2}}.$$

The sine-Gordon equation

The sine-Gordon equation has been used as a mathematical model in many different applications, including the propagation of ultra-short optical pulses in resonant laser media [66], a universal theory of elementary particles [112, 113, 35], and the propagation of magnetic flux in Josephson junctions [59]. Here we consider the classical $(1 + 1)$-dimensional sine-Gordon equation presented in Section 1.2, with parameters $m^2 = c = 1$, and assume that $u(x,t) = \phi(x - vt) = u(\xi)$ is an elementary soliton solution. Then ϕ satisfies the ordinary differential equation $(1 - v^2)\phi_{\xi\xi} - \sin\phi = 0$. Multiplying then by ϕ_x, integrating with respect to ξ and solving for ϕ_ξ, we obtain that

$$\frac{d\phi}{d\xi} = \left(2A - \frac{2\cos\phi}{1 - v^2}\right)^{1/2},$$

where A is the constant of integration. Now we use separation of variables and the substitution $A(1-v^2) = 1$. Integrating both sides and noting that $1 - \cos\phi = 2\sin^2(\frac{1}{2}\phi)$ and noting that the derivative with respect to ϕ of $\ln\tan(\frac{1}{4}\phi)$ equals $\frac{1}{2}\csc(\frac{1}{2}\phi)$, we get

$$\sqrt{2}\ln\left[\frac{\tan(\frac{1}{4}\phi)}{\tan(\frac{1}{4}\phi_0)}\right] = \left[\frac{2}{1 - v^2}\right]^{1/2}(\xi - \xi_0).$$

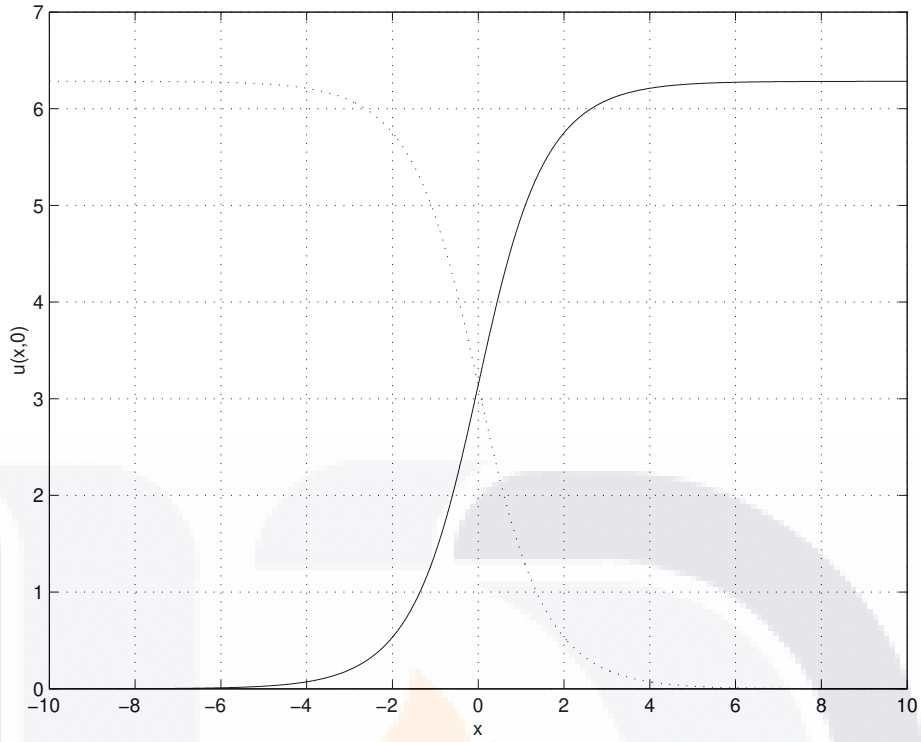

Figure 1.3: Soliton solution (solid line) and anti-soliton solution (dotted line) of the sine-Gordon equation at time 0, with $v = 0.1$.

Finally, solving for ϕ and expressing the result in terms of x and t, it is possible to write the elementary soliton solution as

$$u(x,t) = 4\arctan\left[\exp\left(\frac{x-vt}{\sqrt{1-v^2}}\right)\right].$$

This solution is sometimes called a **kink**; its profile is shown in Figure 1.3. The other soliton solution that can be obtained from the sine-Gordon equation, called the **anti-kink** or **anti-soliton**, is shown in the same figure. Its analytical expression is given by

$$u(x,t) = 4\,\mathrm{arccot}\left[\exp\left(\frac{x-vt}{\sqrt{1-v^2}}\right)\right].$$

We must mention here that the sine-Gordon equation possesses solutions built up from the superposition of solitons and/or anti-solitons. Those solutions and the elementary soliton solutions obtained above are listed in Table 1.1 for the sake of future reference (see [128]).

The Landau-Ginzburg equation

The $(1+1)$-dimensional Landau-Ginzburg equation is another important nonlinear partial differential equation arising in physics that possesses soliton solutions. From the mathematical point of view, the Landau-Ginzburg equation can be seen as a quasilinear Klein-Gordon equation with purely imaginary mass and nonlinear term proportional to u^3. More concretely, the Landau-Ginzburg equation with real parameters m and λ under study in this section can be written as

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} - m^2 u + \lambda u^3 = 0.$$

Using the same technique to find elementary, solitary wave solutions, we suppose that $u(x,t) = \phi(\xi)$, where $\xi = x - vt$ for some $v \in \mathbb{R}$. Then ϕ satisfies the ordinary differential equation

$$(1-v^2)\frac{d^2\phi}{d\xi^2} = -m^2\phi + \lambda\phi^3.$$

Type of solution	Analytical expression
single soliton	$u(x,t) = 4\arctan\left[\exp\left(\dfrac{x-vt}{\sqrt{1-v^2}}\right)\right]$
single anti-soliton	$u(x,t) = u(x,t) = 4\,\mathrm{arccot}\left[\exp\left(\dfrac{x-vt}{\sqrt{1-v^2}}\right)\right]$
two solitons	$u(x,t) = 4\arctan\left[\dfrac{v\sinh(x/\sqrt{1-v^2})}{\cosh(vt/\sqrt{1-v^2})}\right]$
soliton and anti-soliton	$4\arctan\left[\dfrac{\sinh(vt/\sqrt{1-v^2})}{v\cosh(x/\sqrt{1-v^2})}\right]$
"breather"	$u(x,t) = 4\arctan\left[\dfrac{\sqrt{1-v^2}}{v}\dfrac{\sin(vt)}{\cosh(x\sqrt{1-v^2})}\right]$

Table 1.1: Different types of soliton solutions of the sine-Gordon equation.

Solving and then multiplying by $2\phi'(\xi)$, we obtain that

$$\frac{d}{d\xi}\left[\left(\frac{d\phi}{d\xi}\right)^2\right] = \frac{1}{2(1-v^2)}\,\frac{d}{d\xi}\left(\lambda\phi^4 - 2m^2\phi^2\right).$$

We integrate now with respect to ξ both sides of the equation. An integration constant will appear in the right-hand side of the resulting equality. By choosing this constant of integration equal to $m^2/(2\lambda(1-v^2))$, taking the negative square root on both sides of the equation, separating variables, and completing the square in the radical that contains ϕ, we obtain that

$$-\frac{1}{\sqrt{\lambda}}\int_{\phi_0}^{\phi}\frac{d\phi}{\phi^2 - m^2/\lambda} = \int_{\xi_0}^{\xi}\frac{d\xi}{\sqrt{2(1-v^2)}}.$$

Let ξ_0 and ϕ_0 be both equal to zero. Expressing the integrand in the left-hand side of the preceding equality, integrating, and then evaluating from ϕ_0 to ϕ, we get

$$\frac{1}{2m}\ln\left|\frac{(\phi + m/\sqrt{\lambda})(\phi_0 - m/\sqrt{\lambda})}{(\phi - m/\sqrt{\lambda})(\phi_0 + m/\sqrt{\lambda})}\right| = \frac{\xi - \xi_0}{\sqrt{2(1-v^2)}}$$

We choose ϕ_0 and ξ_0 to be equal to zero. Solving then for ϕ we obtain the following soliton (kink) solution for the Landau-Ginzburg equation

$$u(x,t) = \frac{m}{\sqrt{\lambda}} = \tanh\left[\frac{m(x-vt)}{\sqrt{2(1-v^2)}}\right]$$

The corresponding anti-soliton (anti-kink) solution to the Landau-Ginzburg equation is obtained by evaluating the solition solution at $(-x,t)$. A graph showing the kink and anti-kink of the Landau-Ginzburg equation is shown in Figure 1.4.

1.5 Elements of numerical analysis

In our investigation, we are interested in developing finite-difference schemes to approximate radially symmetric solutions of modified nonlinear Klein-Gordon equations. In order to determine how accurate our approximations are, we need to introduce the notions of convergence, consistency and stability. To understand these concepts we must first clarify some ideas from mathematical analysis. Here we follow [105] and [126]. Throughout K denotes the fields $\mathbb{R}$ and $\mathbb{C}$.

Normed linear spaces

A **norm** on a vector space V over a scalar field K is a function $||\cdot||$ that associates every element of V with a real number, such that for any vectors $\bar{u}$ and $\bar{v}$, and any scalar a, the following properties are satisfied:

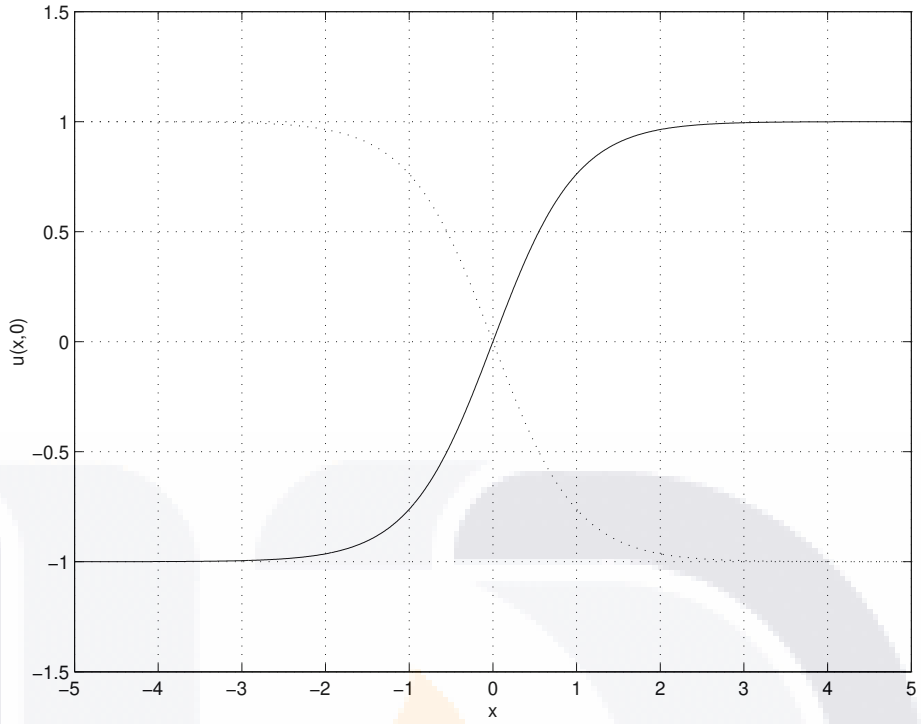

Figure 1.4: Soliton solution (solid line) and anti-soliton solution (dotted line) of the Landau-Ginzburg equation at time 0, with $v = 0.1$.

(i) $||\bar{v}|| \geq 0$, and $||\bar{v}|| = 0$ if and only if $\bar{v} = 0$,

(ii) $||a\bar{v}|| = |a|\ ||\bar{v}||$, and

(iii) $||\bar{u} + \bar{v}|| \leq ||\bar{u}|| + ||\bar{v}||$.

It is worthwhile mentioning that a vector space with a norm associated with it is called a **normed linear space** or simply **normed space**. The following are examples of normed linear spaces with the given norms.

Example 1.5.1. Denote by $|\cdot|$ the standard norm in K. The linear space K^n can be given the **p-norm** ($p \geq 1$)

$$||\bar{x}||_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}.$$

The 1-norm and the 2-norm in K^n are called the the **taxicab norm** and the **Euclidean norm** , respectively. K^n can also be normed by the so called **infinity norm** $||\bar{x}||_\infty = \max\{|x_1|, \ldots, |x_n|\}$. □

Example 1.5.2. Let Δx and p be positive numbers with $p > 1$. The space $\ell_{p,\Delta x}$ is the normed linear space of all infinite sequences $\mathbf{u} = (\ldots, u_{-1}, u_0, u_1, \ldots)$ of elements in K with vector addition and scalar multiplication given componentwise, such that $\sum_{-\infty<j<\infty} |u_j|^p < \infty$. The norm is given by

$$||\mathbf{u}||_{p,\Delta x} = \left(\sum_{k=-\infty}^{\infty} |u_k|^p \Delta x \right)^{1/p}.$$

The space ℓ_p is the space $\ell_{p,1}$. If p is equal to 2 then $\ell_{p,\Delta x}$ is called the **energy space**. □

Example 1.5.3. Let λ represent the Lebesgue measure on $X \subseteq \mathbb{R}$. The space $L_p(X)$ for $p > 1$ is the normed linear space of all equivalence classes of functions $f\colon X \to \mathbb{R}$ under the relation of equivalence

almost everywhere, together with addition and scalar multiplication defined in representatives, such that $\int_X f^p \, d\lambda < \infty$. Its norm is given by

$$||f||_p = \left(\int_X f^p \, d\lambda \right)^{1/p}. \quad \square$$

Example 1.5.4. Let $|| \cdot ||$ be any norm in K^n. The space of all $n \times n$-matrices with coefficients in K is a normed linear space with the usual operations of addition of matrices and scalar multiplication, with **matrix norm** defined by

$$||Q|| = \sup_{||\bar{u}|| \leq 1} \{Q\bar{u}\}. \quad \square$$

Convergence

A difference scheme $L_k^n u_k^n = G_k^n$ approximating the partial differential equation $\mathcal{L}v = F$ is a **convergent** scheme at time t in the norm $|| \cdot ||$ of $\ell_{p,\Delta x}$ if, as $(n+1)\Delta t \to t$,

$$||\mathbf{u}^{n+1} - \mathbf{v}^{n+1}|| \to 0$$

as $\Delta x, \Delta t \to 0$. Here $\mathbf{u}^n = (\dots, u_{-1}^n, u_0^n, u_1^n, \dots)$ and $\mathbf{v}^n = (\dots, v_{-1}^n, v_0^n, v_1^n, \dots)$ are the sequences representing the vector of approximations to the solution of the partial differential equation and the vector of exact solutions whose k-th component is $v(k\Delta x, n\Delta t)$, respectively.

Consistency

The difference scheme $\mathbf{u}^{n+1} = Q\mathbf{u}^n + \Delta t \mathbf{G}^n$ is **consistent** with the partial differential equation $\mathcal{L}v = F$ in the norm $|| \cdot ||$ if the solution v of the differential equation satisfies

$$\mathbf{v}^{n+1} = Q\mathbf{v}^n + \Delta t \mathbf{g}^n + \Delta t \tau^n,$$

and $||\tau^n|| \to 0$ as $\Delta x, \Delta t \to 0$. Moreover, the scheme is said to be accurate with order $\mathcal{O}(\Delta x^p) + \mathcal{O}(\Delta t^q)$ if

$$||\tau^n|| = \mathcal{O}(\Delta x^p) + \mathcal{O}(\Delta t^q).$$

Stability

One interpretation of stability of a finite-difference scheme is that, for a stable scheme, small errors in the initial conditions cause small errors in the solution. As we will see, the definition does allow the errors to grow but limits them to grow no faster than exponential. More precisely, the finite-difference scheme $\mathbf{u}^{n+1} = Q\mathbf{u}^n$ is said to be **stable** with respect to the norm $|| \cdot ||$ if there exist positive constants Δx_0 and Δt_0, and nonnegative constants K and β so that

$$||\mathbf{u}^{n+1}|| \leq K e^{\beta t} ||\mathbf{u}^0||,$$

for $0 \leq t = (n+1)\Delta t$, $0 < \Delta x \leq \Delta x_0$ and $0 < \Delta t \leq \Delta t_0$. If further restrictions on the relationship between Δt and Δx are needed in order to guarantee stability of the finite-difference scheme, we say that the scheme is **conditionally stable**.

One characterization of stability that is often useful comes from the inequality in the definition above. We state this in the following result.

Theorem 1.5.5. *The scheme $\mathbf{u}^{n+1} = Q\mathbf{u}^n$ is stable with respect to the norm $|| \cdot ||$ if and only if there exist positive constants Δx_0 and Δt_0, and nonnegative constants K and β so that*

$$||Q^{n+1}|| \leq K e^{\beta t},$$

for $0 \leq t = (n+1)\Delta t$, $0 < \Delta x \leq \Delta x_0$ and $0 < \Delta t \leq \Delta t_0$. $\square$

The scheme $\mathbf{u}^{n+1} = Q\mathbf{u}^n$ is said to be **stable order** n with respect to the norm $||\cdot||$ if there exist positive constants Δx_0 and Δt_0, and nonnegative constants K_1, K_2 and β such that

$$||\mathbf{u}^{n+1}|| \leq (K_1 + nK_2)e^{\beta t}||\mathbf{u}^0||,$$

for $0 \leq t = (n+1)\Delta t$, $0 < \Delta x \leq \Delta x_0$ and $0 < \Delta t \leq \Delta t_0$. Obviously, if a finite-difference scheme is stable then it will be stable order n. We also realize that the above definition is equivalent to requiring that Q satisfy $||Q^n|| \leq (K_1 + nK_2)e^{\beta t}$.

The use of the discrete Fourier transform is a useful tool in the analysis of stability of finite-difference schemes for initial-value problems. We define the **discrete Fourier transform** of $\mathbf{u} \in \ell_2$ as the function $\hat{u} \in L_2([-\pi, \pi])$ given by

$$\hat{u}(\xi) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} e^{-im\xi} u_m,$$

for $\xi \in [-\pi, \pi]$. The ℓ_2 vectors that we will be using later will be the $\ell_{2,\Delta x}$ vectors that are the solutions to our finite-difference schemes at time step n.

Example 1.5.6. The **central second-order difference** is the linear operator δ^2 that associates with each infinite sequence $\mathbf{u} = (\dots, u_{-1}, u_0, u_1, \dots)$ of real numbers the infinite sequence $\delta^2\mathbf{u}$ whose m-th component is given by $u_{m+1} - 2u_m + u_{m-1}$. It is easy to check that the Fourier transform of $\delta^2\mathbf{u}$ is given by $-4\sin^2\frac{\xi}{2}\hat{u}$. □

It is important to remark that if $\mathbf{u} \in \ell_2$ has discrete Fourier transform $\hat{u}$ then $||\hat{u}||_2 = ||\mathbf{u}||_2$, where the first norm is the L_2-norm on $[-\pi, \pi]$ and the second norm is the ℓ_2-norm. This fact constitutes a bridge between the spaces ℓ_2 and $L_2([-\pi, \pi])$ that provides us with the following important result for stability.

Theorem 1.5.7. *The sequence* $\{\mathbf{u}^n\}$ *is stable in* $\ell_{2,\Delta x}$ *if and only if* $\{\hat{u}^n\}$ *is stable in* $L_2([-\pi, \pi])$. □

Let $\mathbf{u}^{n+1} = Q\mathbf{u}^n$ be a finite difference scheme. Taking discrete Fourier transform in both sides we obtain an equation of the form $\hat{u}^{n+1} = A(\xi)\hat{u}^n$. The matrix $A(\xi)$ is called the **amplification matrix** of the difference scheme. By virtue of Theorem 1.5.7, the stability of the scheme depends on the growth of the amplification matrix raised to the n-th power.

Theorem 1.5.8 (Lax Theorem)**.** *If a two-level difference scheme* $\mathbf{u}^{n+1} = Q\mathbf{u}^n + \Delta t\mathbf{G}^n$ *is consistent in the norm* $||\cdot||$ *to an initial-value problem and is stable with respect to* $||\cdot||$*, the it is convergent with respect to* $||\cdot||$. □

1.6 Finite differences

We could begin by recalling the standard definition of derivative which we have learned in elementary calculus.

Definition 1.6.1. The *derivative* of the function $u(x)$ is defined by the equation

$$u'(x) = \lim_{\Delta x \to 0} \frac{u(x + \Delta x) - u(x)}{\Delta x}. \tag{1.3}$$

provided the limit exists. The number $u'(x)$ is also called the rate of change of u at x.

However, the computers can not handle the previous limit, namely, when $\Delta x \to 0$, and hence a *discrete* analogue of the continuous scenario need to be considered. In the discretization, we can regard that the set of points on which the function is defined is finite, and the function value is available on a discrete set of points. The approximations to the derivative of the function will must to come from these finite sets of points.

Figure 1.5 shows us the discrete set of points x_i where the function is known. We use the notation $u_i = u(x_i)$ to denote the value of the function at the i-th node of the computational grid. We divide the axis into a set of intervals of width $\Delta x_i = x_{i+1} - x_i$. We can fix the grid spacing, it means that all intervals are of equal size, so we will refer to the grid spacing as Δx. If we make the last, we will obtain several advantages when we develop the method as we will see afterward.

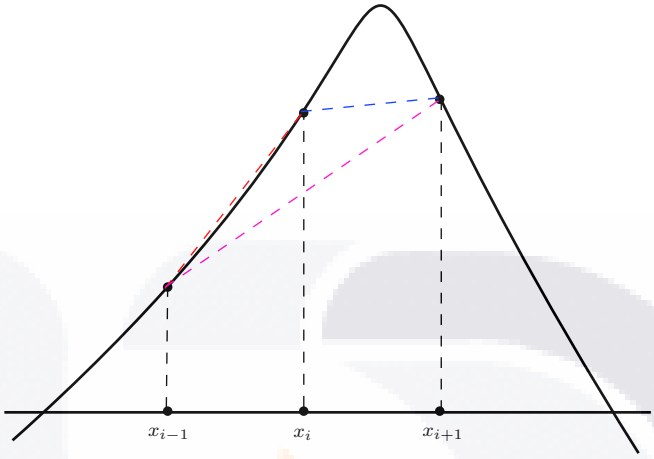

Figure 1.5: Computational grid and example of backward (red dashed line), forward (blue dashed line) and centered (magenta dashed line) linear interpolation to the function.

Finite difference approximation

We employ the definition of derivative in the continuous case to approximate the derivative in the discrete case:

$$u'(x_i) \approx \frac{u(x_i + \Delta x_i) - u(x_i)}{\Delta x} = \frac{u_{i+1} - u_i}{\Delta x}, \tag{1.4}$$

where now Δx is a finite and small but not necessarily infinitesimally small quantity. In the literature, this is known as a *forward Euler* approximation since it uses forward differencing.

Intuitively, we hope that the approximation improves, it means, the error will decrease, as Δx is made smaller. The above is not the only way to approximate the derivative. We provide two other equally valid approximations:

$$u'(x_i) \approx \frac{u(x_i) - u(x_i - \Delta x)}{\Delta x} = \frac{u_i - u_{i-1}}{\Delta x}, \tag{1.5}$$

and

$$u'(x_i) \approx \frac{u(x_i + \Delta x) - u(x_i - \Delta x)}{\Delta x} = \frac{u_{i+1} - u_{i-1}}{\Delta x}. \tag{1.6}$$

Equation (1.5) is known as *backward Euler's* approximation whereas Equation (1.6) represents the *centered difference* approximation. All these definitions are equally equivalent in the continuous case but yield to different approximations in the discrete case. The question becomes which one is better, and is there a way to quantify the error committed. The answer lies in the application of Taylor series analysis.

Taylor series

Let's start with the identity

$$u(x) = u(x_i) + \int_{x_i}^{x} u'(s)\mathrm{d}s. \tag{1.7}$$

Since $u(x)$ is arbitrary, the formula should hold with $u(x)$ replaced by $u'(x)$, it means,

$$u'(x) = u'(x_i) + \int_{x_i}^{x} u''(s)\mathrm{d}s. \tag{1.8}$$

Replacing this expression in the original formula and carrying out the integration (since $u(x_i)$ is constant) we get

$$u(x) = u(x_i) + (x - x_i)u'(x_i) + \int_{x_i}^{x}\int_{x_i}^{x} u''(s)\mathrm{d}s\mathrm{d}s. \tag{1.9}$$

The process can be repeated with

$$u''(x) = u''(x_i) + \int_{x_i}^{x} u'''(s)\mathrm{d}s, \tag{1.10}$$

to get

$$u(x) = u(x_i) + (x - x_i)u'(x_i) + \frac{(x - x_i)^2}{2!}u''(x_i) + \int_{x_i}^{x}\int_{x_i}^{x}\int_{x_i}^{x} u'''\mathrm{d}s\mathrm{d}s\mathrm{d}s. \tag{1.11}$$

We can repeat this process under the assumption that $u(x)$ is sufficiently differentiable, and we find

$$u(x) = u(x_i) + (x - x_i)u'(x_i) + \frac{(x - x_i)^2}{2!}u''(x_i) + \ldots + \frac{(x - x_i)^n}{n!}u^{(n)}(x_i) + R_{n+1}, \tag{1.12}$$

where the remainder is given by

$$R_{n+1} = \int_{x_i}^{x}\cdots\int_{x_i}^{x} u^{(n+1)}(s)(\mathrm{d}s)^{n+1}. \tag{1.13}$$

Equation (1.12) is known as the Taylor series of the function $u(x)$ about the point x_i. Notice that the series is a polynomial in $(x - x_i)$ and the coefficients are the (scaled) derivatives of the function *evaluated* at x_i.

If the $(n+1)$-th derivative of the function u has minimum m and maximum M over the interval $[x_i, x]$ the we can write

$$\int_{x_i}^{x}\cdots\int_{x_i}^{x} m(\mathrm{d}s)^{n+1} \leq R_{n+1} \leq \int_{x_i}^{x}\cdots\int_{x_i}^{x} M(\mathrm{d}s)^{n+1}, \tag{1.14}$$

$$m\frac{(x - x_i)^{n+1}}{(n+1)!} \leq R_{n+1} \leq M\frac{(x - x_i)^{n+1}}{(n+1)!}, \tag{1.15}$$

which shows that the remainder is bounded by the values of the derivative and the distance of the point x to the expansion point x_i raised to the power $n+1$. If we further assume that $u^{(n+1)}$ is continuous then it must take all values between m and M, that is

$$R_{n+1} = u^{(n+1)}(\xi)\frac{(x - x_i)^{n+1}}{(n+1)!}, \tag{1.16}$$

for some $\xi \in [x_i, x]$.

Taylor series and finite differences

The behavior of numerical approximation to differential equations can be studied using Taylor series. First, we consider the forward Euler with Taylor series. For this, we need to expand the function u at x_{i+1} about the point x_i:

$$u(x_i + \Delta x_i) = u(x_i) + \Delta x_i \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x_i^2}{2!}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{\Delta x_i^3}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \ldots \tag{1.17}$$

We can rearrange the Taylor series to get the following

$$\frac{u(x_i + \Delta x_i) - u(x_i)}{\Delta x_i} - \left.\frac{\partial u}{\partial x}\right|_{x_i} = \underbrace{\frac{\Delta x_i}{2!}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{\Delta x_i^2}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \ldots}_{\text{Truncation Error}} \tag{1.18}$$

where it is now clear that the forward Euler formula (1.4) corresponds to truncating the Taylor series after the second term. We can see that the right-hand side of Equation (1.18) coincides with the error committed when we terminate the series and is referred to as the *truncation error*. The truncation error

could be defined as the difference between the partial derivative and its finite difference representation. For sufficiently smooth functions and adequately small Δx_i, the first term in the series is usually used to establish the order of magnitude of the error. The first term in the truncation error is the product of the second derivative evaluated at x_i and the grid spacing Δx_i: the former is a property of the function itself while the latter is a numerical parameter which we can change. Thereby, for finite $\frac{\partial^2 u}{\partial x^2}$, the numerical approximation depends linearly on the parameter Δx_i. If we were to half Δx_i, we would expect a linear decrease in the error, if we make Δx_i sufficiently small. We know that there is a notation to refer this behavior, that is truncation error $\sim \mathcal{O}(\Delta x_i)$. In general, if Δx_i is not constant we choose a representative value of the grid spacing. Note that in general, we can not calculate the exact truncation error; all we can do is characterize the behavior of this error as $\Delta x \to 0$. Thus, we can rewrite Equation (1.18) as

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_i}{\Delta x_i} + \mathcal{O}(\Delta x) \tag{1.19}$$

Now, we can use the Taylor series expansion to obtain an expression for the truncation error when we consider the backward difference formula

$$u(x_i - \Delta x_{i-1}) = u(x_i) - \Delta x_{i-1} \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x_{i-1}^2}{2!} \left.\frac{\partial u^2}{\partial x^2}\right|_{x_i} - \frac{\Delta x_{i-1}^3}{3!} \left.\frac{\partial u^3}{\partial x^3}\right|_{x_i} + \dots \tag{1.20}$$

where $\Delta x_{i-1} = x_i - x_{i-1}$. We proceed to get an expression for the error corresponding to backward difference approximation of the first derivative

$$\frac{u(x_i) - u(x_i - \Delta x_{i-1})}{\Delta x_{i-1}} - \left.\frac{\partial u}{\partial x}\right|_{x_i} = \underbrace{-\frac{\Delta x_{i-1}}{2!} \left.\frac{\partial u^2}{\partial x^2}\right|_{x_i} + \frac{\Delta x_{i-1}^2}{3!} \left.\frac{\partial u^3}{\partial x^3}\right|_{x_i} + \dots}_{\text{Truncation Error}} \tag{1.21}$$

We realize that the truncation error of the backward difference is not the same as the forward difference; it behave similarly in terms of order of magnitude analysis, and is linear in Δx, that is

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_i - u_{i-1}}{\Delta x_{i-1}} + \mathcal{O}(\Delta x) \tag{1.22}$$

Observe that in both cases we used the information provided at just two points to obtain the approximation, and the error performs linearly in both instances.

We can obtain a higher order approximation of the first derivative by combining the two Taylor series Equation (1.17) and (1.20). Notice first that the high order derivatives of the function u are all evaluated at the same point x_i and are the same in both expansions. Now, if we form a linear combination of the equations, the prime error will vanish. Observe Equations (1.18) and (1.21). Multiplying the first by Δx_{i-1} and the second by Δx_i and adding both equations we get:

$$\frac{1}{\Delta x_i + \Delta x_{i-1}} \left[\Delta x_{i-1} \frac{u_{i+1} - u_i}{\Delta x_i} + \Delta x_i \frac{u_i - u_{i-1}}{\Delta x_{i-1}}\right] - \left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{\Delta x_{i-1} \Delta x_i}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{1.23}$$

The approximation uses information about the function u at three points: x_{i-1}, x_i and x_{i+1}. Thus, the truncation error $\sim \mathcal{O}(\Delta x_{i-1} \Delta x_i)$ and is second order. We can observe that on the important case where the grid spacing is constant, the expression simplifies to

$$\frac{u_{i+1} - u_{i-1}}{2\Delta x} - \left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{\Delta x^2}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \dots \tag{1.24}$$

Hence, for an equally spaced grid, the centered difference approximation converges quadratically as $\Delta x \to 0$:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^2) \tag{1.25}$$

Higher order approximation

The Taylor expansion provides a suitable tool to derive a higher order approximation to derivatives of any order. In most of the following we will consider the grid spacing to be constant as is usually the case in most applications. In fact, we will assume constant spacing grid in this thesis.

Equation (1.24) yields the simplest way to derive a fourth order approximation. As an important property of this centered formula is that its truncation error contains only odd derivative terms:

$$\frac{u_{i+1}-u_{i-1}}{2\Delta x}=\frac{\partial u}{\partial x}+\frac{\Delta x^2}{3!}\frac{\partial^3 u}{\partial x^3}+\frac{\Delta x^4}{5!}\frac{\partial^5 u}{\partial x^5}+\frac{\Delta x^6}{7!}\frac{\partial^7 u}{\partial x^7}+\ldots+\frac{\Delta x^{2m}}{(2m+1)!}\frac{\partial^{2m+1} u}{\partial x^{2m+1}}+\ldots \tag{1.26}$$

The above formula can be applied with Δx replace by $2\Delta x$, and $3\Delta x$ respectively, to get:

$$\frac{u_{i+2}-u_{i-2}}{4\Delta x}=\frac{\partial u}{\partial x}+\frac{(2\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3}+\frac{(2\Delta x)^4}{5!}\frac{\partial^5 u}{\partial x^5}+\frac{(2\Delta x)^6}{7!}\frac{\partial^7 u}{\partial x^7}+O(\Delta x^8), \tag{1.27}$$

$$\frac{u_{i+3}-u_{i-3}}{6\Delta x}=\frac{\partial u}{\partial x}+\frac{(3\Delta x)^2}{3!}\frac{\partial^3 u}{\partial x^3}+\frac{(3\Delta x)^4}{5!}\frac{\partial^5 u}{\partial x^5}+\frac{(3\Delta x)^6}{7!}\frac{\partial^7 u}{\partial x^7}+O(\Delta x^8). \tag{1.28}$$

Multiplying Equation (1.26) by 2^2 and subtracting it from Equation (1.27), we cancel the second order error term to get:

$$\frac{8(u_{i+1}-u_{i-1})-(u_{i+2}-u_{i-2})}{12\Delta x}=\frac{\partial u}{\partial x}-\frac{4\Delta x^4}{5!}\frac{\partial^5 u}{\partial x^5}-\frac{20\Delta x^6}{7!}\frac{\partial^7 u}{\partial x^7}+O(\Delta x^8). \tag{1.29}$$

Repeating this process for Equation (1.27) but using the factor 3^2 and subtracting it from Equation (1.28), we get

$$\frac{27(u_{i+1}-u_{i-1})-(u_{i+3}-u_{i-3})}{48\Delta x}=\frac{\partial u}{\partial x}-\frac{9\Delta x^4}{5!}\frac{\partial^5 u}{\partial x^5}-\frac{90\Delta x^6}{7!}\frac{\partial^7 u}{\partial x^7}+O(\Delta x^8). \tag{1.30}$$

Even though both Equation (1.29) and (1.30) are meaningful, the latter is not used in the practice since it does not sense to ignore neighboring points while using more distant ones. Nevertheless, this expresion is appropiate to derive a sixth approximation to the first derivative: multiply equation (1.30) by 9 and the same equation by 4 and subtract to get:

$$\frac{45(u_{i-1}-u_{i-1})-9(u_{i+2}-u_{i-2})+(u_{i+3}-u_{i-3})}{60\Delta x}=\frac{\partial u}{\partial x}+\frac{36\Delta x^6}{7!}\frac{\partial^7 u}{\partial x^7}+O(\Delta x^8). \tag{1.31}$$

The process can be repeated to derive higher order approximations.

2. A structure-preserving method for a fractional wave equation

In this chapter, we consider an initial-boundary-value problem governed by a $(1 + 1)$-dimensional hyperbolic partial differential equation with constant damping that generalizes many nonlinear wave equations from mathematical physics. The model considers the presence of a spatial Laplacian of fractional order which is defined in terms of Riesz fractional derivatives, as well as the inclusion of a generic continuously differentiable potential. It is known that the undamped regime has an associated positive energy functional, and we show here that it is preserved throughout time under suitable boundary conditions. To approximate the solutions of this model, we propose a finite-difference discretization based on fractional centered differences. Some discrete quantities are proposed in this work to estimate the energy functional, and we show that the numerical method is capable of conserving the discrete energy under the same boundary conditions for which the continuous model is conservative. Moreover, we establish suitable computational constraints under which the discrete energy of the system is positive. The method is consistent of second order, and is both stable and convergent. The numerical simulations shown here illustrate the most important features of our numerical methodology.

2.1 Introduction

The design of energy-preserving finite-difference schemes for nonlinear partial differential equations has been an important topic of research since the early studies by L. Vázquez and coworkers in the 1970s. Many nonlinear partial differential equations are known to posses energy functionals that are preserved under suitable boundary conditions, including models like the Schrödinger, the sine-Gordon and the nonlinear Klein–Gordon equations from relativistic quantum mechanics, just to mention some wave equations of physical relevance. Motivated by this fact, several groups of researchers have developed reliable numerical techniques to approximate the solutions of these and other nonlinear conservative systems as well as the constant energy functionals associated to them. The most notable contributions to the state of the art were the energy-preserving finite-difference methodologies proposed for the Schrödinger [119], the sine-Gordon [9, 36] and the nonlinear Klein–Gordon regimes [114]. In fact, those works (among other important papers of those decades) still continue to be sources of motivation for the numerical investigation of nonlinear wave equations [74]. Later on, these studies were extended to account for different potential functions and for dissipative terms. In this way, the investigation of energy- or dissipation-preserving methods was extended to more complicated regimes. At the same time, a solid basis for their design was also formulated by D. Furihata and coworkers in various seminal papers [44, 84]. In many senses, these works constitute the formal birth of the discrete variational derivative method, whose use has been widely accepted in the specialized literature [45].

In general, the use of numerical methods that preserve invariants obeys various physical and mathematical reasons, including the need to establish analytically some numerical properties. On physical grounds, it is highly desirable to have at hand reliable numerical techniques that resemble the dynamics of the continuous models of interest. In that sense, the early reports by L. Vázquez and co-authors [114] communicated the physical need to develop methods with both numerical and meaningful physical properties. Those reports have been perhaps some of the first efforts in the investigation of structure-preserving

methods for partial differential equations or, as R. E. Mickens calls them [86], dynamically consistent numerical techniques. It is worth mentioning that the development of structure-preserving methods has been a fruitful avenue of research in numerical analysis. This approach has been extensively followed in the numerical solution of many partial differential equations of integer order [50, 14, 38, 136, 117]. However, it is known nowadays that various fractional models from physics are also capable of preserving significant quantities. Some examples of such models are some gradient and Hamiltonian extensions of the Hemlholtz conditions for phase space [120], some fractional equivalents of the Fokker–Planck equation for fractal media [120], continuous-limit approximations of systems of coupled oscillators with power-law interactions [63] and mathematical models with fractional dynamics resulting in optimal control theory [40]. In view of the meaningfulness of those problems, some structure-preserving numerical methods have been already proposed to describe the fractional dynamics of those models. For instance, energy-conserving methods have been proposed to approximate the solution of systems consisting of nonlinear fractional Schrödinger equations using finite-differences [131, 132] and Galerkin methods [69].

It is important to note that the notions of 'structure preservation' or 'dynamic consistency' not only refer to the capability of numerical methods to preserve analogues of physical quantities (like energy, momentum, mass, etc.). In a broader sense, these concepts also refer to the capacity of a computational technique to preserve mathematical features of the relevant solutions of continuous systems that naturally arise from the physical context of the problem. A typical example is the condition of positivity (or nonnegativity) of solutions, which is a natural requirement for problems in which the variables of interest are measured in absolute scales [76, 21]. Boundedness is another desirable characteristic in physical problems where there are natural limitations of growth, particularly in models that describe the dynamics of populations under limited resources and space [101, 142] or transport phenomena in turbulent flows. Another mathematical feature of some solutions is the monotonicity, which is important in the approximation of equations whose solution is a cumulative distribution of probability [78] or some traveling wave [77]. In the present work, however, we will consider a nonlinear dissipative wave equation with Riesz space-fractional derivatives for which some positive energy functional is preserved under suitable boundary and parameter conditions. Motivated by the early works by L. Vázquez and D. Furihata, we will design a structure-preserving method that conserves the dissipation of the energy of the system. More concretely, our approach will be based on the use of fractional centered differences, and we will provide discrete schemes for both the solution of the problem and the total energy of the system. We will show here that, under appropriate conditions on the computational parameters, the total energy of the discretized system is likewise a positive function of the time. To that end, various alternative expressions of the energy invariants will be derived. The preserved quantities will be used then to show that the method proposed in this chapter is not only consistent but also stable and convergent of second order. Some simulations will show the capability of the method to preserve the energy under the analytic conditions derived in this work.

This chapter is divided as follows. The nonlinear dissipative wave equation with Riesz space-fractional derivatives that motivates our investigation is presented in Section 2.2, together with the relevant definitions of the fractional differential operators and an energy functional proposed in the literature [5]. We show therein that the initial-boundary-value problem under investigation is a conservative system under suitable analytic conditions. Section 2.3 introduces the discrete nomenclature and the method to solve numerically the problem under investigation. The concept of fractional centered differences will be recalled therein and some useful lemmas will be proved in the way. The most important physical properties of the method will be established in Section 2.4. Concretely, we will establish the capability of the finite-difference scheme to preserve the dissipation or the conservation of energy of the discrete system. In turn, the most important numerical properties of our technique will be proved in Section 2.6. In that stage we will show that our method is a consistent technique, and we will establish the stability and the convergence properties of our scheme. Additionally, that section offers some qualitative simulations that illustrate the capability of our scheme to preserve the energy or the dissipation of energy in Riesz space-fractional wave equations. This work closes with a section of concluding remarks. Additionally, we provide a discussion of the capability of our methodology to preserve the energy of an unbounded system described by a nonlinear Riesz space-fractional wave equation.

2.2 Preliminaries

2.2.1 Long-range interactions

The present section is devoted to provide some physical justification for studying the fractional partial differential equation of (2.7), using properties of systems with linear long-range interactions [124, 123]. Consider a one-dimensional system of interacting oscillators described by the equation of motion

$$\frac{d^s u_n}{dt^s}(t) = I_n(u(t)) + F(u_n(t)), \quad \forall t \in \mathbb{R}^+, \forall n \in \mathbb{Z}. \tag{2.1}$$

In the context of [121], the number s is equal to 1 or 2, the functions u_n represent displacements from the equilibrium and F represents the interaction of the oscillators with an external force. Moreover, the distance between consecutive oscillators is equal to h and the term I_n is defined in general by

$$I_n(u(t)) = \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} J(n,m)\left[u_n(t) - u_m(t)\right], \quad \forall t \in \mathbb{R}^+, \forall n \in \mathbb{Z}. \tag{2.2}$$

Here J represents the interparticle interaction function.

It is important to point out that there are various examples of long-range interactions in physics and other areas of science. A typical example in physics is the linear interaction of particles in a three-dimensional gravitational system [10]. Other examples are the interactions of vortices in two-dimensions, engineering problems on elasticity arising from the study of planar stress, systems of electric charges and systems that consider dipolar forces [15]. Moreover, there are several well-characterized cases of long-range interactions involved in activation and repression of transcription in chromosomal and gene regulation [87]. In various of these examples, the interaction function J satisfies the conditions

(a) $J(n,m) = J(n-m) = J(m-n)$ for all $m, n \in \mathbb{Z}$,

(b) $\sum_{n=1}^{\infty} |J(n)|^2 < \infty$.

It is easy to see that these conditions imply that $J(-n) = J(n)$ for each $n \in \mathbb{Z}$.

Definition 2.2.1 (Tarasov [121])**.** Suppose that conditions (a) and (b) above are satisfied, and let $\alpha > 0$. Then J is called an *α-interaction* if the function

$$J_\alpha(k) = \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} e^{-ikn} J(n) = 2\sum_{n=1}^{\infty} J(n) = \cos(kn), \quad \forall k \in \mathbb{R}, \tag{2.3}$$

satisfies

$$A_\alpha = \lim_{k\to 0} \frac{J_\alpha(k) - J_\alpha(0)}{|k|^\alpha} \in \mathbb{R} \setminus \{0\}. \tag{2.4}$$

Various examples of α-interactions can be found in the appendix of [121]. In the following, we will let $\mathcal{F}_h : u_n(t) \to \hat{u}(k,t)$ denote the Fourier series transform, let $\mathcal{L} : \hat{u}(k,t) \to \tilde{u}(k,t)$ be the passage to the limit when the distance between consecutive oscillators tend to zero, and let $\mathcal{F}^{-1} : \tilde{u}(k,t) \to u(x,t)$ be the inverse Fourier transform. Finally, let $\circ$ represent the composition of functions and define $T = \mathcal{F}^{-1} \circ \mathcal{L} \circ \mathcal{F}_h$. Using these nomenclature, the next theorem establishes conditions under which the partial differential equation of (2.7) can be obtained from systems of oscillators with long-range interactions.

Theorem 2.2.2 (Tarasov [121])**.** *Let $\alpha > 0$ and let J be an α-interaction. Then T transforms the discrete equations of motion* (2.1) *into the fractional continuous equation*

$$\frac{\partial^s u}{\partial t^s}(x,t) - h^\alpha A_\alpha \frac{\partial^\alpha u}{\partial |x|^\alpha}(x,t) - F(u(x,t)) = 0, \quad \forall (x,t) \in \mathbb{R} \times \mathbb{R}^+, \tag{2.5}$$

where the fractional derivative in space is the Riesz fractional derivative of order α.

As a matter of fact [121], a special example of α-interaction is the function defined by $J(n,m) = J_\alpha(n-m)$ for each $m, n \in \mathbb{Z}$ and $1 < \alpha < 2$, where

$$J_\alpha(n) = \frac{(-1)^n \Gamma(\alpha+1)}{\Gamma(\frac{\alpha}{2} - n + 1)\Gamma(\frac{\alpha}{2} + n + 1)}, \quad \forall n \in \mathbb{Z}. \tag{2.6}$$

Use of the transformation T described above results in an approximation of the Riesz spatial derivative. An argument similar to this is employed in [18] to derive the second-order consistent approximation (2.34).

2.2.2 Mathematical model

In this section we let $T > 0$ and $\gamma \in \mathbb{R}^+ \cup \{0\}$, and suppose that $a, b \in \mathbb{R}$ satisfy $a < b$. Throughout this work we will assume that $1 < \alpha \leq 2$ and let $\Omega = (a, b) \times (0, T) \subseteq \mathbb{R}^2$. We will employ here the notation $\overline{\Omega}$ to represent the closure of Ω in $\mathbb{R}^2$ under the standard topology, and will assume that $G : \mathbb{R} \to \mathbb{R}$, that $\phi, \psi : [a, b] \to \mathbb{R}$ and that $f, g : [0, T] \to \mathbb{R}$ are all continuously differentiable functions that satisfy the compatibility conditions $\phi(a) = f(0)$, $\phi(b) = g(0)$, $\psi(a) = f'(0)$ and $\psi(b) = g'(0)$. Moreover, we will suppose that G is nonnegative, that G'' is bounded and that $u : \overline{\Omega} \to \mathbb{R}$ is a sufficiently smooth function that satisfies the initial-boundary-value problem

$$\begin{gathered}\frac{\partial^2 u}{\partial t^2}(x,t) - \frac{\partial^\alpha u}{\partial |x|^\alpha}(x,t) + \gamma \frac{\partial u}{\partial t}(x,t) + G'(u(x,t)) = 0, \quad \forall (x,t) \in \Omega, \\ \text{such that } \begin{cases} u(x,0) = \phi(x), & \forall x \in (a,b), \\ \dfrac{\partial u}{\partial t}(x,0) = \psi(x), & \forall x \in (a,b), \\ u(a,t) = f(t), & \forall t \in (0,T), \\ u(b,t) = g(t), & \forall t \in (0,T), \end{cases}\end{gathered} \tag{2.7}$$

which is a model that results after applying the Fourier series transform, a limiting processes and the inverse Fourier transform to suitable physical systems with long-range interactions (see 2.2.1 for the details). In this work, we define

$$\frac{\partial^\alpha u}{\partial |x|^\alpha}(x,t) = \frac{-1}{2\cos(\frac{\pi\alpha}{2})\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_a^b \frac{u(\xi,t)}{|x-\xi|^{\alpha-1}} d\xi, \quad \forall (x,t) \in \Omega. \tag{2.8}$$

Note that the operator (2.8) is the Riesz fractional derivative of order α in the spatial variable, which is an operator that agrees with the spatial Laplacian when $\alpha = 2$. Alternatively, the Riesz fractional operator can be expressed in terms of the Riemann–Liouville fractional derivatives as

$$\frac{\partial^\alpha u}{\partial |x|^\alpha}(x,t) = -\frac{1}{2\cos(\frac{\pi\alpha}{2})} \left({}_aD_x^\alpha + {}_xD_b^\alpha\right) u(x,t), \quad \forall (x,t) \in \Omega, \tag{2.9}$$

where ${}_aD_x^\alpha$ and ${}_xD_b^\alpha$ are, respectively, the left and the right Riemann–Liouville fractional derivatives in space of order α. More concretely,

$${}_aD_x^\alpha u(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_a^x \frac{u(\xi,t)}{(x-\xi)^{\alpha-1}} d\xi, \quad \forall (x,t) \in \Omega, \tag{2.10}$$

$${}_xD_b^\alpha u(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_x^b \frac{u(\xi,t)}{(\xi-x)^{\alpha-1}} d\xi, \quad \forall (x,t) \in \Omega. \tag{2.11}$$

In the present work, Γ will denote the usual gamma function, namely,

$$\Gamma(z) = \int_0^\infty s^{z-1} e^{-s} ds, \quad \forall s > 0. \tag{2.12}$$

In the following, we will use $L_{x,2}(\overline{\Omega})$ to represent the set of all functions $f : \overline{\Omega} \to \mathbb{R}$ such that $f(\cdot, t) \in L_2([a, b])$ for each $t \in [0, T]$. For each pair $f, g \in L_{x,2}(\overline{\Omega})$, the inner product of f and g is the function of t defined by

$$\langle f, g \rangle_x = \int_a^b f(\xi,t) g(\xi,t) d\xi, \quad \forall t \in [0,T]. \tag{2.13}$$

Here the integration is considered in the sense of Lebesgue. As expected, the Euclidean norm of $f \in L_{x,2}(\overline{\Omega})$ is the function of t defined by $\|f\|_{x,2} = \sqrt{\langle f, f \rangle}$. The set of all functions $f : \overline{\Omega} \to \mathbb{R}$ such that $f(\cdot, t) \in L_1([a, b])$ for each $t \in [0, T]$ will be denoted by $L_{x,1}(\overline{\Omega})$, and for each such f we define its norm as the function of t given by

$$\|f\|_{x,1} = \int_a^b |f(\xi,t)| d\xi, \quad \forall t \in [0,T]. \tag{2.14}$$

The literature on mathematical physics has proposed various functionals to calculate the energy of systems governed by (2.7) when $\gamma = 0$ (see [125], for instance). For purposes of this work, we will use the energy integral employed in [5], which is given by

$$\mathcal{E}(t) = \frac{1}{2}\left\|\frac{\partial u}{\partial t}\right\|_{x,2}^2 + \frac{1}{2}\left\langle u, -\frac{\partial^\alpha u}{\partial |x|^\alpha}\right\rangle_x + \|G(u)\|_{x,1}, \quad \forall t \in [0,T]. \tag{2.15}$$

It is important to note here that the Riesz fractional derivative of order α is a self-adjoint and negative operator [68]. It is a well known fact that positive self-adjoint operators may possess positive square-roots, and that they are unique when they exist (see [41] for a justification of this fact). This and [68] imply that the additive inverse of the Riesz fractional derivative has a square root operator Ξ^α and is unique. Moreover, the following holds for u and v:

$$\left\langle -\frac{\partial^\alpha u}{\partial |x|^\alpha}, v\right\rangle_x = \langle \Xi^\alpha u, \Xi^\alpha v\rangle_x . \tag{2.16}$$

As a consequence, the energy function (2.15) may be rewritten alternatively as

$$\mathcal{E}(t) = \frac{1}{2}\left\|\frac{\partial u}{\partial t}\right\|_{x,2}^2 + \frac{1}{2}\|\Xi^\alpha u\|_{x,2}^2 + \|G(u)\|_{x,1} . \tag{2.17}$$

Obviously, the associated energy density is defined for each $(x,t) \in \Omega$ by

$$\begin{aligned} \mathcal{H}(x,t) &= \frac{1}{2}\left[\frac{\partial u}{\partial t}(x,t)\right]^2 - \frac{1}{2}u(x,t)\frac{\partial^\alpha u}{\partial |x|^\alpha}(x,t) + G(u(x,t)) \\ &= \frac{1}{2}\left[\frac{\partial u}{\partial t}(x,t)\right]^2 + \frac{1}{2}\left[\Xi^\alpha u(x,t)\right]^2 + G(u(x,t)). \end{aligned} \tag{2.18}$$

Here we have used the assumption that G is a nonnegative function.

Theorem 2.2.3. *Let u be a solution of (2.7) with $f = g = 0$ and $\phi(a) = \psi(a) = \phi(b) = \psi(b) = 0$. Then $\mathcal{E}'(t) = -\gamma\|u_t\|_{x,2}^2$, for each $t \in (0,T)$. Here u_t represents the partial derivative of u with respect to t. If additionally $\gamma = 0$ then the system (2.7) is conservative.*

Proof. Beforehand, note that the following identities hold:

$$\frac{1}{2}\frac{d}{dt}\left\|\frac{\partial u}{\partial t}\right\|_{x,2}^2 = \frac{1}{2}\int_a^b \frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t}(\xi,t)\right)^2 d\xi = \left\langle \frac{\partial u}{\partial t}, \frac{\partial^2 u}{\partial t^2}\right\rangle, \tag{2.19}$$

$$\frac{1}{2}\frac{d}{dt}\|\Xi^\alpha u\|_{x,2}^2 = \left\langle \frac{\partial}{\partial t}\left(\Xi^\alpha u\right), \Xi^\alpha u\right\rangle_x = \left\langle \Xi^\alpha\left(\frac{\partial u}{\partial t}\right), \Xi^\alpha u\right\rangle_x = \left\langle \frac{\partial u}{\partial t}, -\frac{\partial^\alpha u}{\partial |x|^\alpha}\right\rangle, \tag{2.20}$$

$$\frac{d}{dt}\|G(u)\|_{x,1} = \int_a^b \frac{\partial}{\partial t}G(u(\xi,t))d\xi = \left\langle \frac{\partial u}{\partial t}, G'(u)\right\rangle. \tag{2.21}$$

Taking derivative with respect to t on both sides of (2.17), using the identities above and the partial differential equation of (2.7), and simplifying algebraically we obtain

$$\mathcal{E}'(t) = \int_a^b \frac{\partial u}{\partial t}(\xi,t)\left[\frac{\partial^2 u}{\partial t^2}(\xi,t) - \frac{\partial^\alpha u}{\partial |x|^\alpha}(\xi,t) + G'(u(\xi,t))\right]d\xi = -\gamma\int_a^b \left[\frac{\partial u}{\partial t}(\xi,t)\right]^2 d\xi, \tag{2.22}$$

whence the result readily follows. □

Corollary 2.2.4. *If u is a solution of (2.7) such that $f = g = 0$ and $\phi(a) = \psi(a) = \phi(b) = \psi(b) = 0$ then*

$$\mathcal{E}(t) = \mathcal{E}(0) - \gamma\int_0^t \left\|\frac{\partial u}{\partial t}\right\|_{x,2}^2 dt, \quad \forall t \in [0,T]. \tag{2.23}$$

Proof. The conclusion is a direct consequence of Theorem 2.2.3. □

In the following sections, we will develop a numerical method to approximate both the solutions of (2.7) and the energy function (2.15) in such way that the discrete versions of Theorem 2.2.3 and Corollary 2.2.4 are still satisfied. Various additional numerical properties of our methodology will be derived in the way, including the positivity of the discrete energy function as well as the consistency, the stability and the convergence of the method.

2.3 Numerical method

For the remainder of this work we let $h > 0$ and τ be fixed step-sizes in space and time, respectively, and assume that $N = T/\tau$ and $M = (b-a)/h$ are positive integers. Consider uniform partitions of $[a, b]$ and $[0, T]$, respectively, given by $x_j = a + jh$ and $t_n = n\tau$ for each $0 \leq j \leq M$ and each $0 \leq n \leq N$. In this work, the symbol v_j^n will represent a numerical approximation to the exact value of $u_j^n = u(x_j, t_n)$, that is, the solution of the initial-boundary-value problem (2.7) at the point (x_j, t_n), for each $0 \leq j \leq M$ and each $0 \leq n \leq N$. Moreover, we will use the discrete linear operators

$$\mu_t u_j^n = \frac{u_j^{n+1} + u_j^n}{2} = u(x_j, t_n) + \mathcal{O}(\tau), \tag{2.24}$$

$$\mu_t^{(1)} u_j^n = \frac{u_j^{n+1} + u_j^{n-1}}{2} = u(x_j, t_n) + \mathcal{O}(\tau^2), \tag{2.25}$$

$$\delta_t u_j^n = \frac{u_j^{n+1} - u_j^n}{\tau} = \frac{\partial u}{\partial t}(x_j, t_n) + \mathcal{O}(\tau), \tag{2.26}$$

$$\delta_t^{(1)} u_j^n = \frac{u_j^{n+1} - u_j^{n-1}}{2\tau} = \frac{\partial u}{\partial t}(x_j, t_n) + \mathcal{O}(\tau^2), \tag{2.27}$$

$$\delta_t^{(2)} u_j^n = \frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{\tau^2} = \frac{\partial^2 u}{\partial t^2}(x_j, t_n) + \mathcal{O}(\tau^2), \tag{2.28}$$

for each $1 \leq j \leq M-1$ and $1 \leq n \leq N-1$. Obviously, the right-hand sides of the equations (2.24)–(2.28) summarize the consistency properties of each discrete operator. In addition, the following operator estimates $G'(u(x_j, t_n))$ with an order of consistency equal to $\mathcal{O}(\tau^2)$:

$$\delta_{u,t}^{(1)} G(u_j^n) = \begin{cases} \dfrac{G(u_j^{n+1}) - G(u_j^{n-1})}{u_j^{n+1} - u_j^{n-1}}, & \text{if } u_j^{n+1} \neq u_j^{n-1}, \\ G'(u_j^n), & \text{if } u_j^{n+1} = u_j^{n-1}. \end{cases} \tag{2.29}$$

It is important to note that the discrete operator (2.29) is clearly well defined. Moreover, the fact that the function G is differentiable at u_j^n for each $1 \leq j \leq M-1$ and each $1 \leq n \leq N-1$ implies that the operator $\delta_{u,t}^{(1)} G$ is continuous at u_j^n. On the other hand, it is worth pointing out that the derivative of G may be approximated using a different definition. For instance, instead of considering differences in the temporal domain in (2.29), one may opt to consider differences with respect to the spatial grid. Consistent approximations for the derivative of G can be derived in that way also, but the author does not know how to propose a numerically efficient and dissipation-preserving technique to solve (2.7) using such approach. On the other hand, use of (2.29) presents the advantage that the rate of change of some discrete energy invariants will result in discrete forms of Theorem 2.2.3 and Corollary 2.2.4 (see Section 2.4).

Definition 2.3.1. For any function $f : \mathbb{R} \to \mathbb{R}$, any $h > 0$ and any $\alpha > -1$ we define the *fractional centered difference* of order α of f at the point x as

$$\Delta_h^\alpha f(x) = \sum_{k=-\infty}^{\infty} g_k^{(\alpha)} f(x - kh), \quad \forall x \in \mathbb{R}, \tag{2.30}$$

whenever the right-hand side of this expression converges. The coefficients of the sequence $(g_k^{(\alpha)})_{k=-\infty}^{\infty}$ are defined by

$$g_k^{(\alpha)} = \frac{(-1)^k \Gamma(\alpha+1)}{\Gamma(\frac{\alpha}{2} - k + 1)\Gamma(\frac{\alpha}{2} + k + 1)}, \quad \forall k \in \mathbb{N} \cup \{0\}. \tag{2.31}$$

For computational purposes, it is convenient to possess an iterative formula to calculate the coefficients of the sequence $(g_k^{(\alpha)})_{k=-\infty}^{\infty}$. Using induction one may readily check that

$$\begin{cases} g_0^{(\alpha)} = \dfrac{\Gamma(\alpha+1)}{\Gamma(\alpha/2+1)^2}, \\ g_{k+1}^{(\alpha)} = \left(1 - \dfrac{\alpha+1}{\alpha/2+k+1}\right) g_k, \quad \forall k \in \mathbb{N} \cup \{0\}. \end{cases} \tag{2.32}$$

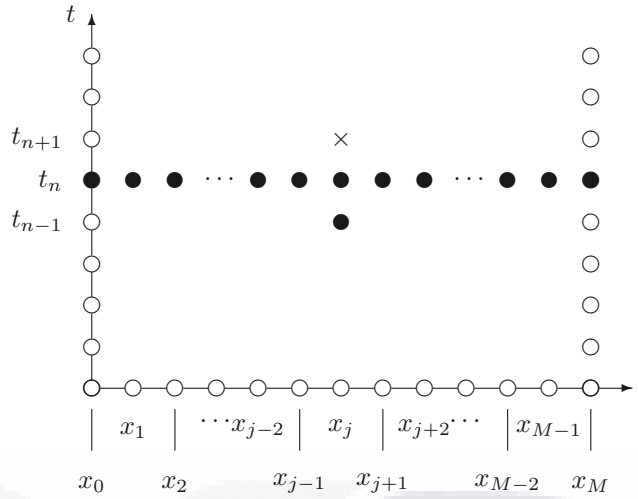

Figure 2.1: Forward-difference stencil for the approximation to the exact solution of (2.7) at the time t_n, using the finite-difference scheme (2.37). The black circles represent the known approximations at the times t_{n-1} and t_n, while the crosses denote the unknown approximations at the time t_{n+1}.

It is important to note also that if $1 < \alpha < 2$ then the fractional centered differences satisfy (see [94])

$$\lim_{h\to 0} \frac{-1}{h^\alpha} \Delta_h^\alpha f(x) = \frac{\partial^\alpha f}{\partial |x|^\alpha}(x), \quad \forall x \in \mathbb{R}. \tag{2.33}$$

We will require the following result from the literature.

Lemma 2.3.2 (Çelik and Duman [18]). *If $1 < \alpha < 2$ then the sequence $(g_k^{(\alpha)})_{k=-\infty}^{\infty}$ satisfies*

(i) $g_0^{(\alpha)} \geq 0$,

(ii) $g_k^{(\alpha)} = g_{-k}^{(\alpha)} < 0$ *for all* $k \geq 1$, *and*

(iii) $\sum_{k=-\infty}^{\infty} g_k^{(\alpha)} = 0$. □

For each nonnegative integer m, let $\mathcal{C}^m(\mathbb{R})$ denote the space of all the functions $f : \mathbb{R} \to \mathbb{R}$ which have continuous derivatives up to the mth order, and let $L_1(\mathbb{R})$ represent the vector space of all the Lebesgue-integrable functions f. As a consequence of Lemma 2.3.2, the series in the right-hand side of (2.30) converges absolutely for any bounded function $f \in L_1(\mathbb{R})$. With this notation, it is easy to see that any $f \in \mathcal{C}^5(\mathbb{R})$ for which all of its derivatives up to order five belong to $L_1(\mathbb{R})$, satisfies the property

$$-\frac{1}{h^\alpha} \Delta_h^\alpha f(x) = \frac{\partial^\alpha f(x)}{\partial |x|^\alpha} + \mathcal{O}(h^2), \quad \forall x \in \mathbb{R}, \tag{2.34}$$

whenever $1 < \alpha < 2$ (see [18]). Under these circumstances, if $1 \leq j \leq M-1$ and $1 \leq n \leq N-1$ then

$$\frac{\partial^\alpha u}{\partial |x|^\alpha}(x_j, t_n) = -\frac{1}{h^\alpha} \sum_{k=-(b-x_j)/h}^{(x_j-a)/h} g_k^{(\alpha)} u(x_j - kh, t_n) + \mathcal{O}(h^2) = \delta_x^{(\alpha)} u_j^n + \mathcal{O}(h^2), \tag{2.35}$$

where

$$\delta_x^{(\alpha)} u_j^n = -\frac{1}{h^\alpha} \sum_{k=0}^{M} g_{j-k}^{(\alpha)} u_k^n. \tag{2.36}$$

With this nomenclature, the finite-difference method to approximate the solution of (2.7) on Ω is given by

$$\begin{gathered} \delta_t^{(2)} v_j^n - \delta_x^{(\alpha)} v_j^n + \gamma \delta_t^{(1)} v_j^n + \delta_{v,t}^{(1)} G(v_j^n) = 0, \quad \forall j \in \{1, \ldots, M-1\}, \forall n \in \{1, \ldots, N-1\}, \\ \text{such that } \begin{cases} v_j^0 = \phi(x_j), & \forall j \in \{1, \ldots, M-1\}, \\ \delta_t v_j^0 = \psi(x_j), & \forall j \in \{1, \ldots, M-1\}, \\ v_0^n = f(t_n), & \forall n \in \{1, \ldots, N-1\}, \\ v_M^n = g(t_n), & \forall n \in \{1, \ldots, N-1\}. \end{cases} \end{gathered} \tag{2.37}$$

Note that this scheme is a three-step method whose forward-difference stencil is shown in Figure 2.1. This technique requires solving an uncoupled system of nonlinear equations at each temporal step. Indeed, note that the only unknown in the jth difference equation of (2.37) is v_j^{n+1}. Consequently, an approximation to the value of the each of the unknowns may be calculated using a numerical method to estimate roots of nonlinear equations. For computational implementation purposes, note that the number v_j^{n+1} is indeed root of

$$F_j^n(v) = (v - v_j^{n-1})(r_+ v + c_j^n) + \tau^2 \left[G(v) - G(v_j^{n-1})\right], \tag{2.38}$$

where

$$r_\pm = 1 \pm \tfrac{1}{2}\tau\gamma, \tag{2.39}$$

$$c_j^n = r_- v_j^{n-1} - 2v_j^n - \tau^2 \delta_x^{(\alpha)} v_j^n. \tag{2.40}$$

Before closing this section, it is important to mention that many fractional problems have been studied using high-order numerical schemes. As examples, some high-order finite-difference schemes were proposed in [145] to approximate the two-dimensional nonlinear space fractional Schrödinger equation, and stable multi-domain spectral penalty methods for Caputo fractional partial differential equations were proposed in [138]. The method introduced in the present work is perhaps one of the first numerically efficient techniques proposed for Riesz space-fractional dissipative wave equations of the Klein–Gordon and sine-Gordon type that has structure-preserving properties. Indeed, we will see in the following sections that (2.37) is a second-order consistent and stable technique which has quadratic order of convergence and for which *a priori* bounds are available. Moreover, in Section 2.4 we will propose energy quantities that mimic the energy properties of the continuous model (2.7). More concretely, discrete forms of Theorem 2.2.3 and Corollary 2.2.4 are available for our finite-difference scheme. Finally, we will show that the energy quantities are positive under suitable conditions on the numerical step-sizes, in agreement with the expression (2.17).

2.4 Energy invariants

In this section we show that the finite-difference method (2.37) satisfies physical properties similar to those satisfied by (2.7). More precisely, we will propose here a numerical energy functional associated to the scheme (2.37) that is preserved under suitable boundary and parameter conditions. For that reason we will suppose that the initial-boundary conditions satisfy

$$\begin{cases} f(t) = g(t) = 0, & \forall t \in [0,T], \\ \phi(x) = \psi(x) = 0, & \text{for } x = a, b. \end{cases} \tag{2.41}$$

Throughout this section, we will employ the spatial mesh

$$R_h = \left\{(x_j)_{j=1}^{M-1} \in \mathbb{R}^{M-1} | x_j = a + jh \text{ for each } 1 \leq j \leq M-1\right\}. \tag{2.42}$$

Let $\mathcal{V}_h$ be the vector space of all real grid functions on R_h. For any $u \in \mathcal{V}_h$ and $j \in \{1, \ldots, M-1\}$ convey that $u_j = u(x_j)$. Moreover, define 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

$$\langle u, v \rangle = h \sum_{j=1}^{M-1} u_j v_j, \tag{2.43}$$

$$\|u\|_1 = h \sum_{j=1}^{M-1} |u_j|, \tag{2.44}$$

for any $u, v \in \mathcal{V}_h$. The Euclidean norm induced by $\langle \cdot, \cdot \rangle$ will be denoted by $\| \cdot \|_2$.

In the following, we will represent the solutions of the finite-difference method (2.37) by $(v^n)_{n=0}^N$, where we convey that $v^n = (v_1^n, \ldots, v_{M-1}^n)$ for each $0 \leq n \leq N$. This convention is justified in view that the identities $v_0^n = v_M^n = 0$ are satisfied in light of (2.41). We will also need the following real matrix of size

$(M-1)\times(M-1)$:

$$A=\begin{pmatrix} g_0^{(\alpha)} & g_{-1}^{(\alpha)} & \cdots & g_{2-M}^{(\alpha)} \\ g_1^{(\alpha)} & g_0^{(\alpha)} & \cdots & g_{3-M}^{(\alpha)} \\ \vdots & \vdots & \ddots & \vdots \\ g_{M-2}^{(\alpha)} & g_{M-3}^{(\alpha)} & \cdots & g_0^{(\alpha)} \end{pmatrix}. \tag{2.45}$$

Definition 2.4.1. A real square matrix A is a *Z-matrix* if all its off-diagonal entries are less than or equal to zero. We say that A is an *M-matrix* or a *Minkowski matrix* if the following are satisfied:

(i) A is a Z-matrix,

(ii) all the diagonal entries of A are positive, and

(iii) there is a diagonal matrix D with positive diagonal entries, such that AD is strictly diagonally dominant.

Among other properties, every M-matrix is nonsingular and the entries of its inverse are all positive numbers (see [42] and references therein). It is worth recalling that this feature of M-matrices has been employed previously in the literature to design non-negativity- and boundedness-preserving implicit numerical methods to approximate the solution of diffusive partial differential equations [78, 77].

Lemma 2.4.2. *The following are properties satisfied by A:*

(a) *A is Hermitian.*

(b) *A is strictly diagonally dominant,*

(c) *All the eigenvalues of A are positive real numbers bounded from above by $2g_0^{(\alpha)}$.*

(d) *A is positive-definite.*

(e) *A is an M-matrix.*

Proof.

(a) Lemma 2.3.2 shows that A is symmetric, so it is Hermitian.

(b) Once again, Lemma 2.3.2 shows that A is strictly diagonally dominant. This readily follows from the fact that for each $j\in\{1,\dots,M-1\}$,

$$R_j=\sum_{\substack{k=1\\k\neq j}}^{M-1}|g_{j-k}^{(\alpha)}|<\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}|g_k^{(\alpha)}|=-\sum_{\substack{k=-\infty\\k\neq 0}}^{\infty}g_k^{(\alpha)}=g_0^{(\alpha)}=|g_0^{(\alpha)}|. \tag{2.46}$$

(c) From (a) we already know that the eigenvalues of A are real. Additionally, the Gershgorin circle theorem guarantees that for each eigenvalue λ of A there exists $1\leq j\leq M-1$ such that $|\lambda-g_0^{(\alpha)}|\leq R_j$, where R_j is given as in (2.46). In particular, this implies that

$$0<g_0^{(\alpha)}-R_j\leq\lambda\leq g_0^{(\alpha)}+R_j<2g_0^{(\alpha)}. \tag{2.47}$$

(d) This follows from the facts that A is Hermitian and that all its eigenvalues are positive.

(e) This property is a consequence of (a) and Lemma 2.3.2. □

Note additionally that if $u,v\in\mathcal{V}_h$ then $\langle u,-\delta_x^{(\alpha)}v\rangle=h^{1-\alpha}u^tAv$. This fact will be required in the next lemma.

Lemma 2.4.3. *There exists a unique linear positive operator $\Lambda^{(\alpha)}:\mathcal{V}_h\to\mathcal{V}_h$ such that*

$$\left\langle -\delta_x^{(\alpha)}u,v\right\rangle=\left\langle \Lambda^{(\alpha)}u,\Lambda^{(\alpha)}v\right\rangle, \tag{2.48}$$

for each $u,v\in\mathcal{V}_h$.

Proof. We provide here a proof different from that given in [132]. The current proof is based on the properties of the sequence $(g_k^{(\alpha)})_{k=-\infty}^{\infty}$. Note firstly that $-\delta_x^{(\alpha)} : \mathcal{V}_h \to \mathcal{V}_h$ is a linear transformation that satisfies the following identities for each $u, v \in \mathcal{V}_h$:

$$\left\langle -\delta_x^{(\alpha)} u, v \right\rangle = h^{1-\alpha} \sum_{j=1}^{M-1} \left(\sum_{k=1}^{M-1} g_{j-k}^{(\alpha)} u_k \right) v_j = h^{1-\alpha} \sum_{k=1}^{M-1} \left(\sum_{j=1}^{M-1} g_{k-j}^{(\alpha)} v_j \right) u_k = \left\langle u, -\delta_x^{(\alpha)} v \right\rangle. \tag{2.49}$$

This means that $-\delta_x^{(\alpha)}$ is a self-adjoint operator on the Hilbert space $\mathcal{V}_h$. Moreover, the fact that the matrix A is positive-definite implies that $\left\langle -\delta_x^{(\alpha)} u, u \right\rangle = h^{1-\alpha} u^t A u \geq 0$ for each $u \in \mathcal{V}$. It follows that $-\delta_x^{(\alpha)}$ has a unique square root operator $\Lambda^{(\alpha)}$, which has the properties of the conclusion of this result. □

The next theorem establishes the existence of invariants for the discrete system (2.37). Beforehand, observe in general that for each $1 \leq n \leq N-1$ the following are satisfied:

$$\begin{aligned} \left\langle \delta_t^{(2)} v^n, \delta_t^{(1)} v^n \right\rangle &= \frac{1}{2\tau^3} \left\langle (v^{n+1} - v^n) - (v^n - v^{n-1}), (v^{n+1} - v^n) + (v^n - v^{n-1}) \right\rangle \\ &= \frac{1}{2\tau^3} \left(\|v^{n+1} - v^n\|_2^2 - \|v^n - v^{n-1}\|_2^2 \right) = \frac{1}{2\tau} \left(\|\delta_t v^n\|_2^2 - \|\delta_t v^{n-1}\|_2^2 \right) \end{aligned} \tag{2.50}$$

and

$$\begin{aligned} \left\langle -\delta_x^{(\alpha)} v^n, \delta_t^{(1)} v^n \right\rangle &= \frac{1}{2\tau} \left[\left\langle -\delta_x^{(\alpha)} v^n, v^{n+1} \right\rangle - \left\langle -\delta_x^{(\alpha)} v^n, v^{n-1} \right\rangle \right] \\ &= \frac{1}{2\tau} \left[\left\langle \Lambda^{(\alpha)} v^n, \Lambda^{(\alpha)} v^{n+1} \right\rangle - \left\langle \Lambda^{(\alpha)} v^{n-1}, \Lambda^{(\alpha)} v^n \right\rangle \right]. \end{aligned} \tag{2.51}$$

Note also that the non-negativity of G yields

$$\begin{aligned} \left\langle \delta_{v,t}^{(1)} G(v^n), \delta_t^{(1)} v^n \right\rangle &= \frac{h}{\tau} \left[\sum_{j=1}^{M-1} \frac{G(v_j^{n+1}) + G(v_j^n)}{2} - \sum_{j=1}^{M-1} \frac{G(v_j^n) + G(v_j^{n-1})}{2} \right] \\ &= \frac{1}{\tau} \left[\mu_t \|G(v^n)\|_1 - \mu_t \|G(v^{n-1})\|_1 \right]. \end{aligned} \tag{2.52}$$

Theorem 2.4.4 (Dissipation of energy)**.** *Let $(v^n)_{n=0}^N$ be solution of the system* (2.37) *under the conditions* (2.41)*. For each $1 \leq n \leq N-1$, let*

$$E^n = \frac{1}{2} \|\delta_t v^n\|_2^2 + \frac{1}{2} \left\langle \Lambda^{(\alpha)} v^n, \Lambda^{(\alpha)} v^{n+1} \right\rangle + \mu_t \left\| G(v^n) \right\|_1. \tag{2.53}$$

If $1 \leq n \leq N-1$ then $\delta_t E^{n-1} = -\gamma \|\delta_t^{(1)} v^n\|_2^2$. In particular, the quantities E^n defined above are invariants of (2.37) *when, in addition, $\gamma = 0$.*

Proof. The proof hinges on Lemma 2.4.3 and the algebraic identities that precede the present theorem. Let Θ^n represent the $(M-1)$-dimensional real vector consisting of the left-hand sides of the difference equations in (2.37) for each $n \in \{1, \ldots, N-1\}$, and suppose that $(v^n)_{n=0}^N$ is a solution of the finite-difference method under the assumptions (2.41). Calculating the inner product of Θ^n with $\delta_t^{(1)} v^n$, using the identities above and collecting terms, we note that

$$\begin{aligned} 0 = \langle \Theta^n, \delta_t^{(1)} v^n \rangle &= \frac{1}{2} \left(\|\delta_t v^n\|_2^2 - \|\delta_t v^{n-1}\|_2^2 \right) + \frac{1}{2} \left(\left\langle \Lambda^{(\alpha)} v^n, \Lambda^{(\alpha)} v^{n+1} \right\rangle - \left\langle \Lambda^{(\alpha)} v^{n-1}, \Lambda^{(\alpha)} v^n \right\rangle \right) \\ &\quad + \left(\mu_t \|G(v^n)\|_1 - \mu_t \|G(v^{n-1})\|_1 \right) + \gamma \left\| \delta_t^{(1)} v^n \right\|_2^2 \\ &= \delta_t E^{n-1} + \gamma \left\| \delta_t^{(1)} v^n \right\|_2^2, \end{aligned} \tag{2.54}$$

whence the conclusion of this result is obtained. If $\gamma = 0$ then $\delta_t E^n = 0$, which implies that the quantities E^n are invariants of (2.37). □

Corollary 2.4.5. *If $(v^n)_{n=0}^N$ is a solution of* (2.37) *when* (2.41) *are satisfied then*

$$E^n = E^0 - \gamma\tau \sum_{k=1}^{n} \left\| \delta_t^{(1)} v^k \right\|_2^2, \quad \forall n \in \{1, \ldots, N-1\}. \tag{2.55}$$

Proof. It readily follows from Theorem 2.4.4. □

Theorem 2.4.4 and Corollary 2.4.5 are clearly the discrete counterparts of Theorem 2.2.3 and Corollary 2.2.4, respectively, and they indicate that our method is a dissipation-preserving technique. Motivated by the fact that the functions (2.17) are nonnegative, we establish now conditions under which the energy invariants (2.53) are also nonnegative. To that end, we will require the following elementary facts will be employed in the sequel without explicit reference:

(A) Note that $|2\langle v, w\rangle| \leq \|v\|_2^2 + \|w\|_2^2$ for any real vectors v and w of the same dimension.

(B) As a consequence, if v and w are real vectors of the same dimension then $\|v \pm w\|_2^2 \leq 2\|v\|_2^2 + 2\|w\|_2^2$.

(C) The properties of the matrix A summarized in Lemma 2.4.2 show that

$$\|\Lambda^{(\alpha)} v\| = \langle v, -\delta_x^{(\alpha)} v\rangle = h^{1-\alpha} v^t A v \leq 2g_0^{(\alpha)} h^{1-\alpha} \|v\|_2^2, \tag{2.56}$$

for any $(M-1)$-dimensional real vector v.

(D) If $(v^n)_{n=0}^N$ is a sequence in $\mathcal{V}_h$ and $1 \leq n \leq N$ then $v^n = v^0 + \tau \sum_{k=0}^{n-1} \delta_t v^k$.

Lemma 2.4.6. *Suppose that $(v^n)_{n=0}^N$ is a solution of (2.37) satisfying (2.41). Then for each $1 \leq n \leq N-1$,*

$$E^n = \frac{1}{2}\|\delta_t v^n\|_2^2 + \frac{1}{2}\mu_t \left\|\Lambda^{(\alpha)} v^n\right\|_2^2 - \frac{\tau^2}{4}\left\|\Lambda^{(\alpha)}\delta_t v^n\right\|_2^2 + \mu_t \|G(v^n)\|_1. \tag{2.57}$$

Moreover, the following energy estimate is satisfied:

$$E^n \geq \frac{1}{2}\left(1 - \frac{\tau^2 g_0^{(\alpha)}}{2h^{\alpha-1}}\right)\|\delta_t v^n\|_2^2 + \mu_t \|G(v^n)\|_1. \tag{2.58}$$

Proof. It is sufficient to show that the sum of the second and the third terms in the right-hand side of (2.57) is equal to $\frac{1}{2}\langle \Lambda^{(\alpha)} v^n, \Lambda^{(\alpha)} v^{n+1}\rangle$. For each $1 \leq n \leq N-1$, observe that

$$\mu_t \left\|\Lambda^{(\alpha)} v^n\right\|_2^2 + \frac{1}{2}\left\langle \Lambda^{(\alpha)} v^n, \Lambda^{(\alpha)}(v^{n+1} - v^n)\right\rangle - \frac{1}{2}\left\langle \Lambda^{(\alpha)} v^{n+1}, \Lambda^{(\alpha)}(v^{n+1} - v^n)\right\rangle = \left\langle \Lambda^{(\alpha)} v^n, \Lambda^{(\alpha)} v^{n+1}\right\rangle, \tag{2.59}$$

whence the identity (2.57) readily follows. As a consequence of this and the inequalities preceding the statement of the present result, it follows that

$$\begin{aligned} \frac{\tau^2}{4}\left\|\Lambda^{(\alpha)}\delta_t v^n\right\|_2^2 &= \frac{1}{8}\left\|\Lambda^{(\alpha)} v^{n+1} - \Lambda^{(\alpha)} v^n\right\|_2^2 + \frac{\tau^2}{8}\left\langle \delta_t v^n, -\delta_x^{(\alpha)}\delta_t v^n\right\rangle \\ &\leq \frac{1}{4}\left[\|\Lambda^{(\alpha)} v^{n+1}\|_2^2 + \|\Lambda^{(\alpha)} v^n\|_2^2\right] + \frac{\tau^2 g_0^{(\alpha)}}{4h^{\alpha-1}}\|\delta_t v^n\|_2^2 \\ &= \frac{1}{2}\mu_t \|\Lambda^{(\alpha)} v^n\|_2^2 + \frac{\tau^2 g_0^{(\alpha)}}{4h^{\alpha-1}}\|\delta_t v^n\|_2^2, \end{aligned} \tag{2.60}$$

for each $1 \leq n \leq N-1$. Using this identity together with the expression (2.57) yields the inequality (2.58). □

The following result establishes conditions under which the quantities (2.53) are nonnegative. This feature of the energy functionals is in agreement with the positive character of its continuous counterpart (2.17). The proof readily follows from the previous lemma.

Theorem 2.4.7 (Positivity of the energy)**.** *Let $(v^n)_{n=0}^N$ be a solution of (2.37) satisfying (2.41), and let $\tau^2 g_0^{(\alpha)} < 2h^{\alpha-1}$. Then the quantities E^n are nonnegative for all $1 \leq n \leq N-1$.*

Proof. The proof readily follows from Lemma 2.4.6. □

Before closing this section, it is important to point out that for each $1 \leq n \leq N-1$, the energy quantity E^n defined in Theorem 2.4.4 has associated the following discrete energy density functions for each $1 \leq j \leq M-1$:

$$H_j^n = \frac{1}{2}\left(\delta_t v_j^n\right)^2 - \frac{1}{2} v_j^n \delta_x^{(\alpha)} v_j^{n+1} + \mu_t G(v_j^n) = \frac{1}{2}\left(\delta_t v_j^n\right)^2 + \frac{1}{2}\Lambda^{(\alpha)} v_j^n \Lambda^{(\alpha)} v_j^{n+1} + \mu_t G(v_j^n). \tag{2.61}$$

2.5 Unbounded domains

In the present section we discuss briefly the case when the problem (2.7) is defined on an unbounded spatial-temporal domain. To that end, we let $\Omega = \mathbb{R} \times \mathbb{R}^+ \subset \mathbb{R}^2$. Suppose that $G : \mathbb{R} \to \mathbb{R}$ is continuously differentiable, and that $\phi, \psi : [a, b] \to \mathbb{R}$ are all infinitely smooth functions on $\mathbb{R}$ that decrease rapidly. Let $u : \overline{\Omega} \to \mathbb{R}$ be a sufficiently smooth function that satisfies the initial-value problem

$$\begin{gathered} \frac{\partial^2 u}{\partial t^2}(x,t) - \frac{\partial^\alpha u}{\partial |x|^\alpha}(x,t) + \gamma \frac{\partial u}{\partial t}(x,t) + G'(u(x,t)) = 0, \quad \forall (x,t) \in \Omega, \\ \text{such that } \begin{cases} u(x,0) = \phi(x), & \forall x \in (a,b), \\ \dfrac{\partial u}{\partial t}(x,0) = \psi(x), & \forall x \in (a,b). \end{cases} \end{gathered} \tag{2.62}$$

To approximate the solutions of (2.62), we consider a regular spatial partition on $\mathbb{R}$ of the form $x_j = jh$ for each $j \in \mathbb{Z}$, where $h > 0$ is the partition norm. Similarly, we consider a partition of the temporal domain of the form $t_n = n\tau$ for each $n \in \mathbb{N} \cup \{0\}$, where $\tau > 0$ is the temporal step-size. Under these circumstances, the spatial mesh is

$$R_h = \left\{ (x_j)_{j=-\infty}^{\infty} \in \mathbb{R}^\omega \,|\, x_j = jh \text{ for each } j \in \mathbb{Z} \right\}. \tag{2.63}$$

We use $\mathcal{V}_h$ to denote the real vector space of grid functions on R_h. Moreover, if $u \in \mathcal{V}_h$ then we use u_j to denote the number $u(x_j)$. The symbol $\ell^p(R_h)$ will denote the classical spaces of integrable functions with domain R_h for each $p \geq 1$. The usual norm of $\ell^p(R_h)$ will be represented by $\|\cdot\|_p$, and the inner product of $\ell^2(R_h)$ will be denoted by $\langle \cdot, \cdot \rangle$.

Note that the series in the right-hand side of (2.30) converges absolutely for any function $f \in \ell^1(R_h)$. This fact readily follows from Lemma 2.3.2. As a consequence, for each $u \in \ell^1(R_h)$ we can define the discrete space-fractional difference operator of order α of u at x_j as

$$\delta_x^{(\alpha)} u_j = -\frac{1}{h^\alpha} \sum_{k=-\infty}^{\infty} g_{j-k}^{(\alpha)} u_k, \quad \forall j \in \mathbb{Z}. \tag{2.64}$$

It is easy to check that $\delta_x^{(\alpha)}$ is a linear operator on $\ell^1(R_h)$. With this notation, the finite-difference method to approximate the solution of (2.62) is given by

$$\begin{gathered} \delta_t^{(2)} u_j^n - \delta_x^{(\alpha)} u_j^n + \gamma \delta_t^{(1)} u_j^n + \delta_{u,t}^{(1)} G(u_j^n) = 0, \quad \forall j \in \mathbb{Z}, \forall n \in \mathbb{N}, \\ \text{such that } \begin{cases} u_j^0 = \phi(x_j), & \forall j \in \mathbb{Z}, \\ \delta_t u_j^0 = \psi(x_j), & \forall j \in \mathbb{Z}. \end{cases} \end{gathered} \tag{2.65}$$

The following is an extension of Lemma 2.3.2.

Lemma 2.5.1. *There exists a unique linear positive operator $\Lambda^{(\alpha)} : \ell^1(R_h) \to \ell^1(R_h)$ such that*

$$\left\langle -\delta_x^{(\alpha)} u, v \right\rangle = \left\langle \Lambda_h^\alpha u, \Lambda_h^\alpha v \right\rangle, \quad \forall u, v \in \ell^1(R_h). \tag{2.66}$$

Proof. Again, our proof will be different from that provided in [132]. Note firstly that for each $u, v \in \ell^1(R_h) \subseteq \ell^2(R_h)$, the sequences $-\delta_x^{(\alpha)} u$ and $-\delta_x^{(\alpha)} v$ belong to $\ell^2(R_h)$, which means that both $\left\langle -\delta_x^{(\alpha)} u, v \right\rangle$ and $\left\langle u, -\delta_x^{(\alpha)} v \right\rangle$ exist in $\mathbb{R}$. On the other hand, using the properties of the coefficients $(g_k^{(\alpha)})_{k=-\infty}^{\infty}$ summarized in Lemma 2.3.2 we note that

$$\left\langle -\delta_x^{(\alpha)} u, v \right\rangle = \frac{1}{h^{1-\alpha}} \sum_{j=-\infty}^{\infty} \left(\sum_{k=-\infty}^{\infty} g_{j-k}^{(\alpha)} u_k \right) v_j = \frac{1}{h^{1-\alpha}} \sum_{k=-\infty}^{\infty} \left(\sum_{j=-\infty}^{\infty} g_{k-j}^{(\alpha)} v_j \right) u_k = \left\langle u, -\delta_x^{(\alpha)} v \right\rangle, \tag{2.67}$$

for all $u, v \in \ell^1(R_h)$. This means that $-\delta_x^{(\alpha)}$ is a self-adjoint operator, and we only need to show now that it is also positive. To that end let $u \in \ell^1(R_h)$ and define the real vector $\bar{u}^M = (u_{-M}, \ldots, u_{-1}, u_0, u_1, \ldots, u_M)$ of dimension $2M + 1$, for each $M \in \mathbb{M}$. Also, define the real matrix A^M of size $(2M+1) \times (2M+1)$ by

$$\bar{A}^M = \begin{pmatrix} g_0^{(\alpha)} & g_{-1}^{(\alpha)} & \cdots & g_{-2M}^{(\alpha)} \\ g_1^{(\alpha)} & g_0^{(\alpha)} & \cdots & g_{1-2M}^{(\alpha)} \\ \vdots & \vdots & \ddots & \vdots \\ g_{2M}^{(\alpha)} & g_{2M-1}^{(\alpha)} & \cdots & g_0^{(\alpha)} \end{pmatrix}. \tag{2.68}$$

From the previous sections we know that each of these matrices is positive-definite and, in particular, it follows that $(\bar{u}^M)^t \bar{A}^M \bar{u}^M \geq 0$ for each $M \in \mathbb{N}$. As a consequence,

$$\begin{aligned}\left\langle -\delta_x^{(\alpha)} u, u \right\rangle &= h^{1-\alpha} \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} g_{j-k}^{(\alpha)} u_k u_j = h^{1-\alpha} \lim_{M\to\infty} \sum_{j=-M}^{M} \sum_{k=-M}^{M} g_{j-k}(\alpha) u_k u_j \\ &= h^{1-\alpha} \lim_{M\to\infty} \bar{u}^M \bar{A}^M \bar{u}^M \geq 0,\end{aligned} \tag{2.69}$$

for each $u \in \ell^1(R_h)$. As a consequence, there exists a unique linear and positive square root $\Lambda^{(\alpha)} : \ell^1(R_h) \to \ell^1(R_h)$ which satisfies the properties of the lemma. □

The proof of the following result is now similar to that of Theorem 2.4.4.

Theorem 2.5.2 (Energy property). *Let $(v^n)_{n=0}^{\infty} \subseteq \ell^1(R_h)$ be a solution of (2.65), and define the constants E^n through (2.53) for each $n \in \mathbb{N}$. Then the constants satisfy $\delta_t E^{n-1} = -\gamma \|\delta_t^{(1)} v^n\|_2^2$ for each $n \in \{1, \ldots, N-1\}$. As a consequence, the quantities E^n are invariants of (2.65) when $\gamma = 0$.* □

2.6 Numerical results

The main numerical properties of the finite-difference method (2.37) as well as some illustrative computational simulations are presented in this stage. Here we show that our scheme is a consistent, stable and convergent technique under suitable conditions on the parameters of the model. In a first stage, we show that (2.37) is a second-order consistent technique. For practical purposes we define the following continuous and discrete functionals:

$$\mathcal{L}u(x,t) = \frac{\partial^2 u}{\partial t^2}(x,t) - \frac{\partial^\alpha u}{\partial |x|^\alpha}(x,t) + \gamma \frac{\partial u}{\partial t}(x,t) + G'(u(x,t)), \quad \forall (x,t) \in \Omega, \tag{2.70}$$

$$Lu_j^n = \delta_t^{(2)} u_j^n - \delta_x^{(\alpha)} u_j^n + \gamma \delta_t^{(1)} u_j^n + \delta_{u,t}^{(1)} G(u_j^n), \quad \forall j \in \{1, \ldots, M-1\}, \forall n \in \{1, \ldots, N-1\}. \tag{2.71}$$

Theorem 2.6.1 (Consistency). *If $u \in \mathcal{C}_{x,t}^{5,4}(\overline{\Omega})$ then there exists a constant $C > 0$ which is independent of h and τ such that for each $j \in \{1, \ldots, M-1\}$ and each $n \in \{1, \ldots, N-1\}$,*

$$\left| Lu_j^n - \mathcal{L}u(x_j, t_n) \right| \leq C(\tau^2 + h^2). \tag{2.72}$$

Proof. We employ here the usual argument with Taylor polynomials and the identity (2.35). Using the hypotheses of continuous differentiability, there exist constants $C_1, C_2, C_3, C_4 \in \mathbb{R}$ such that

$$\left| \delta_t^{(2)} u_j^n - \frac{\partial^2 u}{\partial t^2}(x_j, t_n) \right| \leq C_1 \tau^2, \tag{2.73}$$

$$\left| \delta_x^{(\alpha)} u_j^n - \frac{\partial^\alpha u}{\partial |x|^\alpha}(x_j, t_n) \right| \leq C_2 h^2, \tag{2.74}$$

$$\left| \delta_t^{(1)} u_j^n - \frac{\partial u}{\partial t}(x_j, t_n) \right| \leq C_3 \tau^2, \tag{2.75}$$

$$\left| \delta_{u,t}^{(1)} G(u_j^n) - G'(u(x_j, t_n)) \right| \leq C_4 \tau^2, \tag{2.76}$$

for each $j \in \{1, \ldots, M-1\}$ and each $n \in \{1, \ldots, N-1\}$. The conclusion of this theorem is readily reached using the triangle inequality and defining $C = \max\{C_1, C_2, \gamma C_3, C_4\}$. □

The following result will be useful to establish a priori bounds for the solution of (2.37), and to prove the stability and convergence properties of (2.37). It is obviously a discrete version of the well-known Gronwall inequality.

Lemma 2.6.2 (Pen-Yu [95]). *Let $(\omega^n)_{n=0}^N$ and $(\rho^n)_{n=0}^N$ be finite sequences of nonnegative mesh functions, and suppose that there exists $C \geq 0$ such that*

$$\omega^n \leq \rho^n + C\tau \sum_{k=0}^{n-1} \omega^k. \tag{2.77}$$

Then $\omega^n \leq \rho^n e^{Cn\tau}$ for each $0 \leq n \leq N$. □

Theorem 2.6.3. *If $(v^n)_{n=0}^N$ is a solution of (2.37) satisfying (2.41) and $8Tg_0^{(\alpha)}\tau < h^{\alpha-1}$ then there exists $C \in \mathbb{R}^+$ such that*

$$\|v^n\|_2^2 \leq 4\left(\|v^0\|_2^2 + 2T^2E_0\right)e^{Cn\tau}, \quad \forall n \in \{1,\dots,N\}. \tag{2.78}$$

Proof. Note firstly that $8Tg_0^{(\alpha)}\tau < h^{\alpha-1}$ implies that $\tau^2 g_0^{(\alpha)} < 2h^{\alpha-1}$. Theorem 2.4.7 guarantees then that the quantities E^n are nonnegative and that $E^n \leq E_0$ for each $1 \leq n \leq N$. Let $C \in \mathbb{R}^+$ satisfy

$$\frac{4Tg_0^{(\alpha)}}{h^{\alpha-1}}\left(\frac{2}{C}+\tau\right) < 1. \tag{2.79}$$

It is easy to check that $2\eta < C\tau(1-\eta)$ where $\eta = 4T\tau g_0^{(\alpha)}h^{1-\alpha}$. Using these facts and the remarks before Lemma 2.4.6 together with the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned}
\|v^n\|_2^2 &\leq 2\|v^0\|_2^2 + 2n\tau^2\sum_{k=0}^{n-1}\|\delta_t v^k\|_2^2 \\
&\leq 2\|v^0\|_2^2 + 4T\tau\sum_{k=0}^{n-1}\left[\frac{1}{2}\|\delta_t v^k\|_2^2 + \frac{1}{2}\mu_t\|\Lambda^{(\alpha)}v^k\|_2^2 + \mu_t\|G(v^k)\|_1\right] \\
&\leq 2\|v^0\|_2^2 + 4T^2E^0 + T\tau^3\sum_{k=0}^{n-1}\|\Lambda^{(\alpha)}\delta_t v^k\|_2^2 \\
&\leq 2\|v^0\|_2^2 + 4T^2E^0 + \left(\frac{4Tg_0^{(\alpha)}}{h^{\alpha-1}}\right)\tau\sum_{k=0}^{n-1}\left[\|v^{k+1}\|_2^2 + \|v^k\|_2^2\right],
\end{aligned} \tag{2.80}$$

for each $1 \leq n \leq N$. Collecting all the terms with $\|v^n\|_2^2$ and dividing by $1-\eta$ we reach

$$\|v^n\|_2^2 \leq C_1\left(\|v^0\|_2^2 + 2T^2E^0\right) + C_2\tau\sum_{k=0}^{n-1}\|v^k\|_2^2, \quad \forall n \in \{1,\dots,N\}, \tag{2.81}$$

where $C_1 = 2(1-\eta)^{-1}$ and $C_2 = 2\eta\tau^{-1}(1-\eta)^{-1}$. The conclusion of this result is reached now using Lemma 2.6.2 after noting that $C_1 < 4$ and $C_2 < C$. □

Lemma 2.6.4. *Let $G \in \mathcal{C}^2(\mathbb{R})$ and $G'' \in L^\infty(\mathbb{R})$, and suppose that $(u^n)_{n=0}^N$, $(v^n)_{n=0}^N$ and $(R^n)_{n=0}^N$ are sequences in $\mathbb{R}^{M-1}$. Let $\epsilon^n = v^n - u^n$ and $\widetilde{G}^n = \delta_{v,t}G(v^n) - \delta_{w,t}G(w^n)$ for each $0 \leq n \leq N$. Then there exists $C_1 \in \mathbb{R}^+$ that depends only on G such that*

$$|2\langle R^n - \widetilde{G}^n, \delta_t^{(1)}\varepsilon^n\rangle| \leq 2\|R^n\|_2^2 + C_1\left(\|\varepsilon^{n+1}\|_2^2 + \|\varepsilon^{n-1}\|_2^2 + \|\delta_t\varepsilon^n\|_2^2 + \|\delta_t\varepsilon^{n-1}\|_2^2\right). \tag{2.82}$$

Moreover, there exist $C_2, C_3 \in \mathbb{R}^+$ that depend only on G such that for each $1 \leq k \leq N-1$,

$$2\tau\left|\sum_{n=1}^{k}\langle R^n - \widetilde{G}^n, \delta_t^{(1)}\varepsilon^n\rangle\right| \leq 2\tau\sum_{n=0}^{k}\|R^n\|_2^2 + C_2\|\varepsilon^0\|_2^2 + C_3\tau\sum_{n=0}^{k}\|\delta_t\varepsilon^n\|_2^2. \tag{2.83}$$

Proof. Let $C_0 = \sup\{G''(u) : u \in \mathbb{R}\}$. As a consequence of the Mean Value Theorem and a straightforward integration we obtain that $|\widetilde{G}_j^n| \leq C_0(|\varepsilon_j^{n+1}| + |\varepsilon_j^{n-1}|)$ for each $1 \leq j \leq M-1$ and each $1 \leq n \leq N-1$. It follows that

$$\begin{aligned}
|2\langle R^n - \widetilde{G}^n, \delta_t^{(1)}\varepsilon^n\rangle| &\leq 2\|R^n\|_2^2 + 2\|\widetilde{G}^n\|_2^2 + \|\delta_t^{(1)}\varepsilon^n\|_2^2 \\
&\leq 2\|R^n\|_2^2 + 4C_0\left(\|\varepsilon^{n+1}\|_2^2 + \|\varepsilon^{n-1}\|_2^2\right) + \frac{1}{2}\left(\|\delta_t\varepsilon^n\|_2^2 + \|\delta_t\varepsilon^{n-1}\|_2^2\right),
\end{aligned} \tag{2.84}$$

whence the inequality (2.82) readily follows with $C_1 = \max\{4C_0, \frac{1}{2}\}$. Using that inequality and the remarks

before Lemma 2.4.6 we obtain that

$$\begin{aligned}
2\tau\left|\sum_{n=1}^{k}\langle R^n-\widetilde{G}^n,\delta_t^{(1)}\varepsilon^n\rangle\right| &\leq 2\tau\sum_{n=0}^{k}\|R^n\|_2^2+2C_1\tau\left[\sum_{n=0}^{k+1}\|\varepsilon^n\|_2^2+\sum_{n=0}^{k}\|\delta_t\varepsilon^n\|_2^2\right]\\
&\leq 2\tau\sum_{n=0}^{k}\|R^n\|_2^2+2C_1\tau\left[\sum_{n=0}^{k+1}\left(2\|\varepsilon^0\|_2^2+2T\tau\sum_{l=0}^{n-1}\|\delta_t\varepsilon^l\|_2^2\right)+\sum_{n=0}^{k}\|\delta_t\varepsilon^n\|_2^2\right]\\
&\leq 2\tau\sum_{n=0}^{k}\|R^n\|_2^2+4C_1T\|\varepsilon^0\|_2^2+2C_1(2T^2+1)\tau\sum_{n=0}^{k}\|\delta_t\varepsilon^n\|_2^2,
\end{aligned}\tag{2.85}$$

for each $1\leq k\leq N-1$. The conclusion of this result follows for $C_2=4C_1T$ and $C_3=2C_1(2T^2+1)$. □

We turn our attention to the stability and the convergence properties of (2.37). In the following results, the constants C_1, C_2 and C_3 are as in the previous lemma, and (ϕ_v,ψ_v,f,g) and (ϕ_w,ψ_w,f,g) will denote two sets of initial-boundary conditions of (2.7).

Theorem 2.6.5 (Stability)**.** *Let $G\in\mathcal{C}^2(\mathbb{R})$ and $G''\in L^\infty(\mathbb{R})$, and suppose that $\tau,h\in\mathbb{R}^+$ satisfy*

$$\frac{\tau^2 g_0^{(\alpha)}}{2h^{\alpha-1}}+C_3\tau<1.\tag{2.86}$$

Let $\mathbf{v}=(v^n)_{n=0}^N$ and $\mathbf{w}=(w^n)_{n=0}^N$ be solutions of (2.37) for (ϕ_v,ψ_v,f,g) and (ϕ_w,ψ_w,f,g), respectively, and let $\varepsilon^n=v^n-w^n$ for each $0\leq n\leq N$. Then there exist $C_4,C_5\in\mathbb{R}^+$ independent of $\mathbf{v}$ and $\mathbf{w}$ such that

$$\|\delta_t\varepsilon^n\|_2^2\leq C_4\left(\|\delta_t\varepsilon^0\|_2^2+\mu_t\|\Lambda^{(\alpha)}\varepsilon^0\|_2^2+\|\epsilon^0\|_2^2\right)e^{C_5n\tau},\quad \forall n\in\{1,\ldots,N-1\}.\tag{2.87}$$

Proof. Beforehand, let $\eta_0\in\mathbb{R}^+$ satisfy

$$\frac{\tau^2 g_0^{(\alpha)}}{2h^{\alpha-1}}<\eta_0<1-C_3\tau.\tag{2.88}$$

Obviously, the sequence $(\varepsilon^n)_{n=0}^N$ satisfies the initial-boundary-value problem

$$\begin{gathered}
\delta_t^{(2)}\varepsilon_j^n-\delta_x^{(\alpha)}\varepsilon_j^n+\gamma\delta_t^{(1)}\varepsilon_j^n+\delta_{v,t}^{(1)}G(v_j^n)-\delta_{w,t}G(w_j^n)=0,\quad \forall j\in\{1,\ldots,M\},\forall n\in\{1,\ldots,N\},\\
\text{such that }\begin{cases}\varepsilon_j^0=\phi_v(x_j)-\phi_w(x_j), & \forall j\in\{1,\ldots,M-1\},\\ \delta_t\varepsilon_j^0=\psi_v(x_j)-\psi_w(x_j), & \forall j\in\{1,\ldots,M-1\},\\ \varepsilon_0^n=\varepsilon_M^n=0, & \forall n\in\{1,\ldots,N-1\}.\end{cases}
\end{gathered}\tag{2.89}$$

For the sake of convenience, let $\widetilde{G}_j^n=\delta_{v,t}^{(1)}G(v_j^n)-\delta_{w,t}G(w_j^n)$ for each $1\leq j\leq M-1$ and each $1\leq n\leq N-1$. From the identities preceding Theorem 2.4.4 and the proof of Lemma 2.4.6, we readily obtain that

$$\left\langle\delta_t^{(2)}\varepsilon^n,\delta_t^{(1)}\varepsilon^n\right\rangle=\frac{1}{2\tau}\left(\|\delta_t\varepsilon^n\|_2^2-\|\delta_t\varepsilon^{n-1}\|_2^2\right),\tag{2.90}$$

$$\langle-\delta_x^{(\alpha)}\varepsilon^n,\delta_t^{(1)}\varepsilon^n\rangle=\delta_t\left(\frac{1}{2}\mu_t\|\Lambda^{(\alpha)}\varepsilon^{n-1}\|_2^2-\frac{\tau^2}{4}\|\Lambda^{(\alpha)}\delta_t\varepsilon^{n-1}\|_2^2\right),\tag{2.91}$$

$$|2\langle\widetilde{G}^n,\delta_t^{(1)}\varepsilon^n\rangle|\leq C_1\left(\|\delta_t\varepsilon^n\|_2^2+\|\delta_t\varepsilon^{n-1}\|_2^2+\|\varepsilon^{n+1}\|_2^2+\|\varepsilon^{n-1}\|_2^2\right),\tag{2.92}$$

for each $1\leq n\leq N-1$ and for some $C_1\in\mathbb{R}^+$. Let $k\in\{1,\ldots,N-1\}$. Taking the inner product of $\delta_t^{(1)}\epsilon_j^n$ with both sides of the respective difference equation of (2.89), substituting the identities above, calculating then the sum of the resulting identity for all $n\in\{1,\ldots,k\}$, multiplying by 2τ on both sides, applying Lemma 2.6.4 with $R^n=0$ and simplifying algebraically we obtain

$$\begin{aligned}
(1-\eta_0)\|\delta_t\varepsilon^k\|_2^2\leq\left(1-\frac{\tau^2 g_0^{(\alpha)}}{2h^{\alpha-1}}\right)\|\delta_t\varepsilon^k\|_2^2&\leq\|\delta_t\varepsilon^k\|_2^2+\mu_t\|\Lambda^{(\alpha)}\varepsilon^k\|_2^2-\frac{\tau^2}{2}\|\Lambda^{(\alpha)}\delta_t\varepsilon^k\|_2^2\\
&=\|\delta_t\varepsilon^0\|_2^2+\mu_t\|\Lambda^{(\alpha)}\varepsilon^0\|_2^2-\frac{\tau^2}{2}\|\Lambda^{(\alpha)}\delta_t\varepsilon^0\|_2^2-2\tau\sum_{n=1}^{k}\left[\gamma\|\delta_t^{(1)}\varepsilon^n\|_2^2+\langle\widetilde{G}^n,\delta_t^{(1)}\varepsilon^n\rangle\right]\\
&\leq\|\delta_t\varepsilon^0\|_2^2+\mu_t\|\Lambda^{(\alpha)}\varepsilon^0\|_2^2+C_2\|\varepsilon^0\|_2^2+C_3\tau\sum_{n=0}^{k}\|\delta_t\varepsilon^n\|_2^2.
\end{aligned}\tag{2.93}$$

Subtracting $C_3\tau\|\delta_t\varepsilon^k\|_2^2$ on both ends of this inequality and dividing next both sides by $1-\eta_0-C_3\tau$, it follows that there exist constants $C_4, C_5 \in \mathbb{R}^+$ such that

$$\|\delta_t\varepsilon^k\|_2^2 \leq C_4\left(\|\delta_t\varepsilon^0\|_2^2 + \mu_t\|\Lambda^{(\alpha)}\varepsilon^0\|_2^2 + \|\varepsilon^0\|_2^2\right) + C_5\tau\sum_{n=0}^{k-1}\|\delta_t\varepsilon^n\|_2^2. \tag{2.94}$$

The conclusion of this theorem is reached now using Lemma 2.6.2. □

It is worth noting that the inequality (2.86) is satisfied for sufficiently small values of τ. Finally, we tackle the problem of the convergence of the numerical method (2.37). The proof of the following result is similar to that of Theorem 2.6.5, for that reason we provide only an abridged proof.

Theorem 2.6.6 (Convergence)**.** *Let $u \in \mathcal{C}_{x,t}^{5,4}(\overline{\Omega})$ be a solution of (2.7) with $G \in \mathcal{C}^2(\mathbb{R})$ and $G'' \in L^\infty(\mathbb{R})$, and let $(v^n)_{n=0}^N$ be a solution of (2.37) for the initial-boundary conditions (ϕ, ψ, f, g). Assume that (2.41) hold, and let $\epsilon^n = v^n - u^n$ for each $0 \leq n \leq N$. If (2.86) holds then the method (2.37) is convergent of order $\mathcal{O}(\tau^2 + h^2)$.*

Proof. Let $\eta_0 \in \mathbb{R}^+$ be as in the proof of Theorem 2.6.5, and let R_j^n be the truncation error at the point (x_j, t_n) for each $0 \leq j \leq M$ and each $1 \leq n \leq N$. Then $(\epsilon^n)_{n=0}^N$ satisfies

$$\begin{gathered}\delta_t^{(2)}\epsilon_j^n - \delta_x^{(\alpha)}\epsilon_j^n + \gamma\delta_t^{(1)}\epsilon_j^n + \delta_{v,t}^{(1)}G(v_j^n) - \delta_{w,t}G(w_j^n) = R_j^n, \quad \forall j \in \{1,\ldots,M-1\}, \forall n \in \{1,\ldots,N-1\}, \\ \text{such that } \begin{cases} \epsilon_j^0 = \delta_t\epsilon_j^0 = 0, & \forall j \in \{1,\ldots,M-1\}, \\ \epsilon_0^n = \epsilon_M^n = 0, & \forall n \in \{1,\ldots,N-1\}. \end{cases}\end{gathered} \tag{2.95}$$

Following the proof of Theorem 2.6.5, let $\widetilde{G}_j^n = \delta_{v,t}^{(1)}G(v_j^n) - \delta_{w,t}G(w_j^n)$ for each $1 \leq j \leq M-1$ and each $1 \leq n \leq N-1$. Proceeding as in the proof of that theorem, we readily obtain

$$\begin{aligned}(1-\eta_0)\|\delta_t\epsilon^k\|_2^2 &\leq \|\delta_t\epsilon^0\|_2^2 + \mu_t\|\Lambda^{(\alpha)}\epsilon^0\|_2^2 + 2\tau\sum_{n=1}^{k}\langle R^n - \widetilde{G}^n, \delta_t^{(1)}\epsilon^n\rangle \\ &\leq \|\delta_t\epsilon^0\|_2^2 + \mu_t\|\Lambda^{(\alpha)}\epsilon^0\|_2^2 + C_2\|\epsilon^0\|_2^2 + 2\tau\sum_{n=0}^{k}\|R^n\|_2^2 + C_3\tau\sum_{n=0}^{k}\|\delta_t\epsilon^n\|_2^2,\end{aligned} \tag{2.96}$$

for each $1 \leq k \leq M-1$. Subtracting $C_3\tau\|\delta_t\epsilon^k\|_2^2$ on both ends of this inequality and dividing both sides by $1-\eta_0-C_3\tau$, it follows that there exist constants $C_4, C_5 \in \mathbb{R}^+$ such that

$$\|\delta_t\epsilon^k\|_2^2 \leq C_4\left(\|\delta_t\epsilon^0\|_2^2 + \mu_t\|\Lambda^{(\alpha)}\epsilon^0\|_2^2 + \|\epsilon^0\|_2^2 + \tau\sum_{n=0}^{k}\|R^n\|_2^2\right) + C_5\tau\sum_{n=0}^{k}\|\delta_t\epsilon^n\|_2^2. \tag{2.97}$$

Let C be the constant of Lemma 2.6.4, and let $C_6 = C_4C^2e^{C_5T}T$. Lemmas 2.6.4 and 2.6.2, and the initial-boundary conditions in (2.95) imply now that $\|\delta_t\epsilon^k\|_2^2 \leq C_6(\tau^2+h^2)$, whence the conclusion follows. □

Finally, we provide some numerical approximations of the solution of problem (2.7) that show the capability of (2.37) to preserve the energy. In our implementation of Newton's method, the initial approximation to the root of F_j^n will be the number v_j^n. In all our numerical experiments, we will prescribe the initial data using a suitable exact solution of a nonlinear wave equation with derivatives of integer order. For all our simulations we will use a tolerance equal to 1×10^{-8} and a maximum number of iterations equal to 20.

Example 2.6.7. Let $0 < \omega < 1$. In this example, we let $G(u) = 1-\cos u$ for all $u \in \mathbb{R}$, and use the exact solution of the classical sine-Gordon equation described by

$$u(x,t) = 4\arctan\left(\frac{\sqrt{1-\omega^2}\cos\omega t}{\omega\cosh\sqrt{1-\omega^2}x}\right), \quad \forall (x,t) \in \mathbb{R}\times(\mathbb{R}^+\cup\{0\}). \tag{2.98}$$

Computationally, we consider the domain $\Omega = (-30,30)\times(0,100)$, $h = 0.5$ and $\tau = 0.05$. Figure 2.2 shows the numerical solution (left column) and the associated Hamiltonian (right column) of the problem (2.7) obtained using (2.37) and (2.61), respectively, for $\omega = 0.9$ and $\gamma = 0$. Various derivative orders were

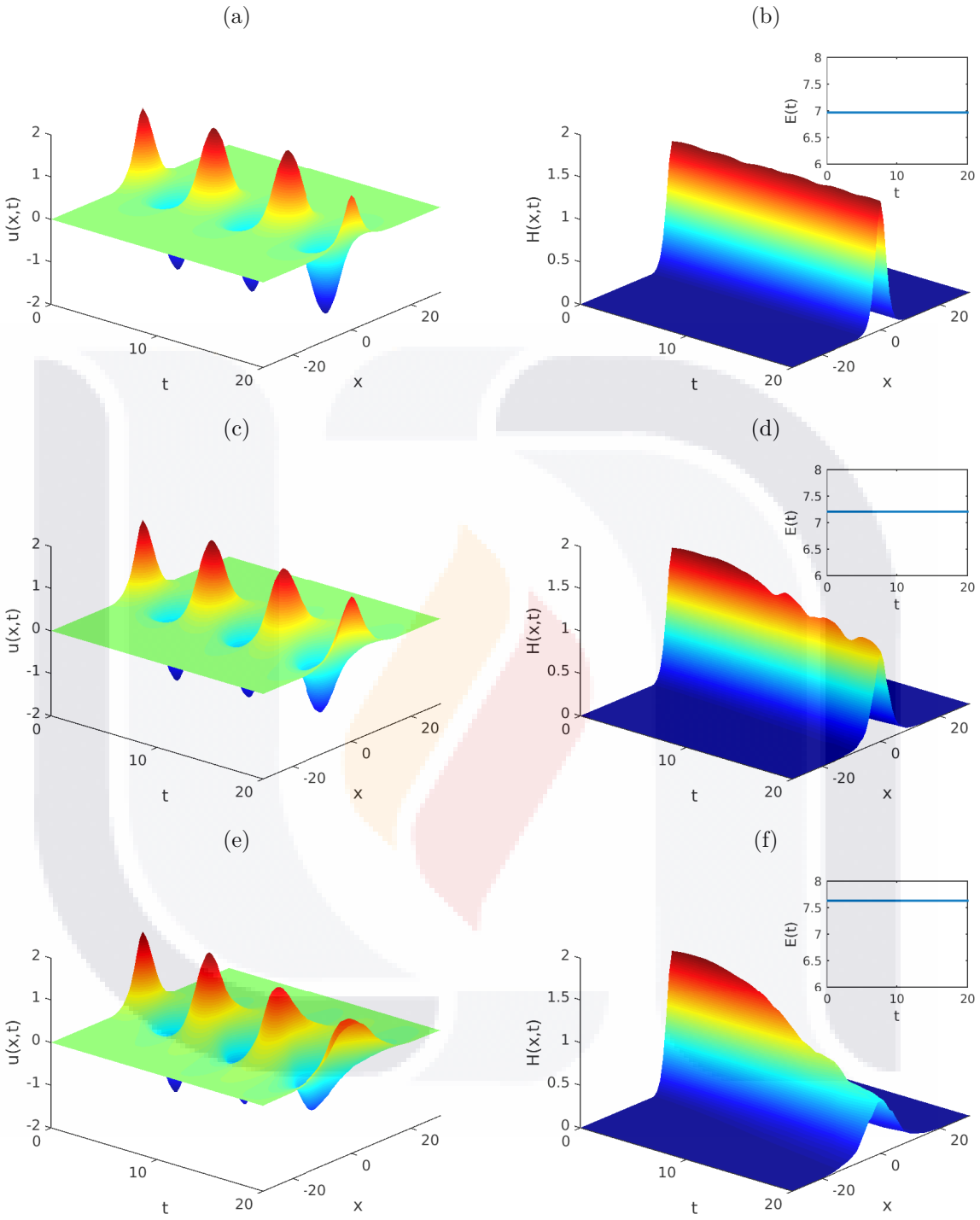

Figure 2.2: Graphs of the numerical solution (left column) and the associated Hamiltonian (right column) of the problem (2.7) with $G(u) = 1 - \cos u$ obtained using (2.37) and (2.61) on $\Omega = (-30, 30) \times (0, 100)$. The initial data were provided by (2.98) with $\omega = 0.9$, and the parameters employed were $\gamma = 0$, $h = 0.5$ and $\tau = 0.05$. Various derivative orders were used, namely, $\alpha = 2$ (top row), $\alpha = 1.6$ (middle row) and $\alpha = 1.2$ (bottom row). The insets of the graphs of the right column represent the discrete dynamics of the total energy (2.53) of the system.

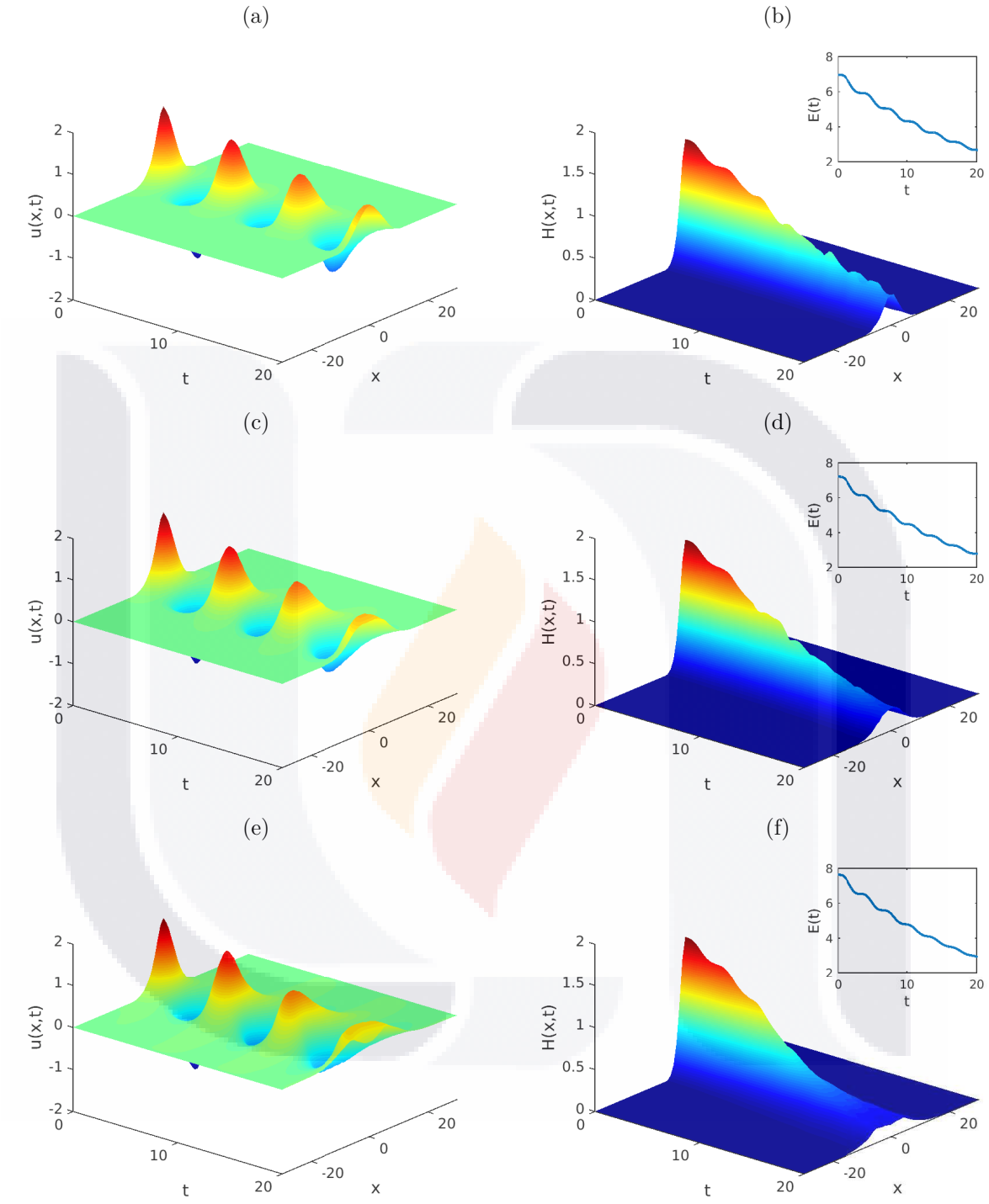

Figure 2.3: Graphs of the numerical solution (left column) and the associated Hamiltonian (right column) of the problem (2.7) with $G(u) = 1 - \cos u$ obtained using (2.37) and (2.61) on $\Omega = (-30, 30) \times (0, 100)$. The initial data were provided by (2.98) with $\omega = 0.9$, and the parameters employed were $\gamma = 0.05$, $h = 0.5$ and $\tau = 0.05$. Various derivative orders were used, namely, $\alpha = 2$ (top row), $\alpha = 1.6$ (middle row) and $\alpha = 1.2$ (bottom row). The insets of the graphs of the right column represent the discrete dynamics of the total energy (2.53) of the system.

used, namely, $\alpha = 2$ (top row), $\alpha = 1.6$ (middle row) and $\alpha = 1.2$ (bottom row). The insets of the graphs of the right column represent the discrete dynamics of the total energy (2.53) of the system. The results show that the discrete total energy is conserved. We have used different computational parameters and the result (not shown here in view of their redundancy) show that the discrete total energy is likewise conserved, in agreement with Theorem 2.4.4. □

Example 2.6.8. Consider now the same problem as in Example 2.6.7, but letting $\gamma = 0.05$. The results of the simulations are shown in Figure 2.3. Obviously, in this case the quantities E^n are not conserved in view of the presence of a nonzero damping term. These results are in agreement with Theorem 2.4.4. □

Before we close this section, we must point out that the simulations were obtained using an implementation of our method in ©Matlab 8.5.0.197613 (R2015a) on a ©Sony Vaio PCG-5L1P laptop computer with Kubuntu 16.04 as operating system. In terms of computational times, we are aware that better results may be obtained with more modern equipment and more modest Linux/Unix distributions.

3. An efficient method for a fractional inhibitor-activator system

Departing from a two-dimensional hyperbolic system that describes the interaction between some activator and inhibitor substances in chemical reactions, we investigate a general form of that model using a finite-difference approach. The model under investigation is a nonlinear system consisting of two coupled partial differential equations with generalized reaction terms. The presence of two-dimensional diffusive terms consisting of fractional operators of the Riesz type is considered here, using spatial differentiation orders in the set $(0,1) \cup (1,2]$. We impose initial conditions on a closed and bounded rectangle, and a finite-difference methodology based on the use of fractional centered differences is proposed. Among the most important results of this work, we prove the existence and the uniqueness of the solutions of the numerical method, and establish analytically the second-order consistency of our scheme. Moreover, the discrete energy method is employed to prove the stability and the quadratic convergence of the technique. Some numerical simulations obtained through our method show the appearance of Turing patterns and wave instabilities, in agreement with some reports found in the literature on superdiffusive hyperbolic activator-inhibitor systems. As a new application, we show that Turing patterns are also present in subdiffusive scenarios.

3.1 Introduction

The investigation on the conditions under which Turing patterns appear in physical systems has been a highly transited avenue of research from the mathematical, the numerical and the physical points of view. It is well know that many nonlinear systems exhibit Turing patterns under suitable conditions on the parameters of the model and the initial data. Some diffusion-reaction systems exhibit the presence of patterns, like some coupled systems which describe the interaction between inhibitor and activator substances in chemistry [31, 28], especially in chemical reactions with chlorine dioxide, iodine, and malonic acid [106]. In fact, several different Turing patterns are also found in the chlorine-iodide-malonic acid reaction, including hexagonal, striped [107], and oscillatory structures [139]. Outside the chemical sciences, there is also evidence on the presence of this kind of nonlinear behavior. For instance, there is experimental evidence on the presence of azimuthal Turing patterns in Kerr combs generated by whispering-gallery-mode resonators [23], and the theory suggests that diffusion-reaction systems may be used to understand the formation of this type of patterns in biology [62]. Even the labyrinthine structure of the cerebral cortex has been identified as a complex three-dimensional Turing pattern [16]. Moreover, it is well known that the Brusselator is a system which exhibits the presence of that type of structures [96, 12].

The physical models described in the paragraph above are diffusive equations. It is well known that these systems have the physical limitation that any perturbation is instantaneously propagated throughout the system. For that reason, hyperbolic forms of these equations are physically preferred. It turns out that a wide variety of Turing patterns have been found also in hyperbolic systems. For example, Turing instabilities have been investigated in diffusive predator-prey models with hyperbolic mortality [118, 144], in hyperbolic models for locally interacting cell systems [75], in the hyperbolic chaos of standing wave patters generated by a modulated pump source [54] and in the spreading of infectious diseases in hyperbolic susceptible-infected-removed models [7]. Also, the presence of various wave and Turing patterns has been

studied in the context of hyperbolic forms of the Brusselator [22, 3], in some hyperbolic models for self-organized biological aggregations and movement [32], in network systems through collective patterns and single differentiated nodes [135], in predator-prey reaction-diffusion models with spatiotemporal delays [137] and in hyperbolic vegetation models for semiarid environments [24], just to mention some systems.

In recent years, fractional derivatives have been introduced to mathematical models in order to provide more realistic descriptions of the physical phenomena. For instance, many fractional systems have been obtained as the continuous limit of discrete systems of particles with long-range interactions [121, 125]. However, independently of that, fractional derivatives have been successfully used in the theory of viscoelasticity [60], the theory of thermoelasticity [100], financial problems under a continuous time frame [109], self-similar protein dynamics [49] and quantum mechanics [90]. Moreover, some distributed-order fractional diffusion-wave equations are used in the modeling of groundwater flow to and from wells [115, 98]. As expected, the complexity of fractional problems is considerably higher that that of integer-order models, whence the need to design reliable numerical techniques to approximate the solutions is pragmatically justified. In this direction, the literature reports on various methods to approximate the solutions of fractional systems. For example, some numerical methods have been proposed to solve fractional partial differential equations using fractional centered differences [80, 82], the time-fractional diffusion equation [6], the fractional Schrödinger equation in multiple spatial dimensions [11], the nonlinear fractional Korteweg-de Vries–Burgers equation [34], the fractional FitzHugh–Nagumo monodomain model in two spatial dimensions [72], distributed-order time-fractional diffusion-wave equations on bounded domains [140] and some Hamiltonian hyperbolic fractional differential equations that generalize various well-known wave equations from relativistic quantum mechanics [79].

In light of these facts, the investigation on the presence of Turing patterns in fractional systems (in both the parabolic and hyperbolic types) has been also an interesting topic of research in recent years. Some reports have studied the presence of these patterns in simple models with fractional diffusion [67], in fractional reaction-diffusion systems with indices of different order [46] and with multiple homogeneous states [27], in hyperbolic inhibitor-activator systems with fractional diffusion [89], in two-species fractional reaction-diffusion systems [52] and in reaction models with sub-diffusion [93]. At the same time, various numerical methods have been proposed in the literature to investigate complex nonlinear models [56, 65, 134]. Motivated by these facts, the purpose of this work is to investigate numerically a two-dimensional hyperbolic system with superdiffusion that describes the interaction between an activator and an inhibitor in chemical reactions. For convenience, we will study a generalized form of the physical model, and provide a discretization of this system using fractional centered differences. Using some properties of fractional discrete operators and a fixed-point theorem, we will establish the existence (and, ultimately, the uniqueness also) of solutions of the numerical method. By employing the standard argument with Taylor polynomials, we will show that the method is a second-order consistent technique. The discrete energy method will be employed then to prove the stability and the convergence properties of our technique. Some computational experiments will be carried out in order to verify the validity of our code and to propose an application to subdiffusive systems.

This chapter is sectioned as follows. In Section 3.2, we provide the mathematical model under investigation, which is a system of hyperbolic partial differential equations with fractional diffusion in two spatial dimensions. Some sufficient conditions for the presence of Turing patterns are recalled therein, and the generalized form of the physical model is provided. In that section, we also introduce the concept of fractional centered differences, which is the cornerstone to approximate the terms with fractional diffusion. We will record therein some useful properties on fractional centered differences for the sake of convenience. Section 3.3 is devoted to provide the discrete nomenclature and the numerical method to approximate the solutions of our generalized model. In that section, we also establish that the numerical technique is solvable and provide comments on its computer implementation. The most interesting numerical features of our technique are established in Section 3.4. More precisely, we show that the method is a quadratically consistent method, which is stable and quadratically convergent. As a corollary, we will notice that our scheme has a unique solution under suitable parameter conditions. Section 3.5 provides some computer simulations. As an application of our technique, we exhibit the presence of Turing patters in various scenarios. The results will be in qualitative agreement with predictions reported in the specialized literature. We close this work with a section of concluding remarks, and an appendix in which we provide the proofs for the technical lemmas employed.

3.2 Preliminaries

Suppose that $a_1, a_2, b_1, b_2 \in \mathbb{R}$ satisfy $a_1 < b_1$ and $a_2 < b_2$, and let $T > 0$. Let $B = (a_1, b_1) \times (a_2, b_2)$ and define $\Omega = B \times (0, T)$. We will employ $\overline{B}$ and $\overline{\Omega}$ to represent respectively the closures of B and Ω under the standard topology of $\mathbb{R}^3$, and we will use ∂B to denote the boundary of B. In this chapter, $u, v : \overline{\Omega} \to \mathbb{R}$ represent functions and let $x = (x_1, x_2)$. Throughout, we will assume that $u(x,t) = v(x,t) = 0$, for each $t \in [0,T]$ and $x \in \mathbb{R}^2 \setminus \overline{B}$.

Definition 3.2.1 (Macías-Díaz [81])**.** Let $\alpha > -1$, let $u : \overline{\Omega} \to \mathbb{R}$ be any function, and suppose that n is a nonnegative integer such that $n - 1 < \alpha \leq n$. The *Riesz fractional derivatives* of u of order α with respect to x_1 and with respect to x_2 at the point (x,t) are defined, respectively, by

$$\frac{\partial^\alpha u(x,t)}{\partial |x_1|^\alpha} = \frac{-1}{2\cos(\frac{\pi\alpha}{2})\Gamma(n-\alpha)} \frac{\partial^n}{\partial x_1^n} \int_{-\infty}^{\infty} \frac{u(\xi, x_2, t)d\xi}{|x_1 - \xi|^{\alpha+1-n}}, \quad \forall (x,t) \in \Omega, \tag{3.1}$$

$$\frac{\partial^\alpha u(x,t)}{\partial |x_2|^\alpha} = \frac{-1}{2\cos(\frac{\pi\alpha}{2})\Gamma(n-\alpha)} \frac{\partial^n}{\partial x_2^n} \int_{-\infty}^{\infty} \frac{u(x_1, \xi, t)d\xi}{|x_2 - \xi|^{\alpha+1-n}}, \quad \forall (x,t) \in \Omega. \tag{3.2}$$

Here, Γ is the usual Gamma function.

Definition 3.2.2 (Macías-Díaz [81])**.** Let $\alpha > -1$ and assume that n is a nonnegative integer such that $n - 1 < \alpha \leq n$. The *Riesz fractional Laplacian* of order α of the function $u : \overline{\Omega} \to \mathbb{R}$ at the point (x,t) is given by

$$\nabla^\alpha u(x,t) = \frac{\partial^\alpha u(x,t)}{\partial |x_1|^\alpha} + \frac{\partial^\alpha u(x,t)}{\partial |x_2|^\alpha}, \quad \forall (x,t) \in \Omega. \tag{3.3}$$

It is worth pointing out that the classical second-order derivatives of u with respect to x_1 and x_2 result from (3.1) and (3.2), respectively, in the case when $\alpha = 2$. Moreover, notice that the right-hand side of (3.3) becomes the classical Laplacian in the spatial variables in that case.

For the remainder of this work, we will use α_1 and α_2 to represent real numbers in $(0,1) \cup (1,2]$. Assume that a, b, c, d_u, d_v are nonnegative numbers, suppose that τ_u, τ_v are positive and let $\phi^u, \phi^v, \psi^u, \psi^v : \overline{B} \to \mathbb{R}$. The functions ϕ^u and ϕ^v denote the initial profiles for u and v, respectively, and ψ^u and ψ^v are the respective initial velocities. With these conventions, the problem under consideration in this work is the following nonlinear initial-value problem, which describes the hyperbolic dynamics of an activator-inhibitor system with anomalous diffusion:

$$\begin{aligned}
\tau_u \frac{\partial^2 u(x,t)}{\partial t^2} + \frac{\partial u(x,t)}{\partial t} &= u(x,t) - av(x,t) + bu(x,t)v(x,t) - [u(x,t)]^3 + d_u \nabla^{\alpha_1} u(x,t), \quad \forall (x,t) \in \Omega, \\
\tau_v \frac{\partial^2 v(x,t)}{\partial t^2} + \frac{\partial v(x,t)}{\partial t} &= u(x,t) - cv(x,t) + d_v \nabla^{\alpha_2} v(x,t), \quad \forall (x,t) \in \Omega, \\
&\text{such that } \begin{cases} u(x,0) = \phi^u(x), & \forall x \in B, \\ v(x,0) = \phi^v(x), & \forall x \in B. \\ \dfrac{\partial u}{\partial t}(x,0) = \psi^u(x), & \forall x \in B, \\ \dfrac{\partial v}{\partial t}(x,0) = \psi^v(x), & \forall x \in B. \end{cases}
\end{aligned} \tag{3.4}$$

The system (3.4) describes the spatio-temporal dynamics of interaction between an activator substance and an inhibitor, each of them represented by u and v, respectively. In this context, the constants τ_u and τ_v are the inertial times of u and v, respectively, and d_u and d_v are the respective diffusion coefficients. It is worthwhile to note that this model has been presented here in dimensionless form. The reaction terms of the partial differential equations of (3.4) were first proposed in the literature to describe the chlorine-iodine-malonic acid reaction [31]. Indeed, the model in [31] is obtained from (3.4) letting $\tau_u = \tau_v = 0$, $d_u = 1$, $d_v = d \in \mathbb{R}^+$ and $\alpha_1 = \alpha_2 = 2$. Moreover, the problem (3.4) was studied in [89] using $\tau_u = \tau_v = \tau \in \mathbb{R}^+$, $d_u = 1$, $d_v = d$, $\alpha_1 = \alpha$, $\alpha_2 = \beta$ and $\alpha, \beta \in (1,2]$. In that case, it was established that some sufficient parametric conditions for the presence of Turing patterns are provided by

$$1 < c < a < a_T, \quad d > 1, \quad b < \sqrt{c(a-c)}, \tag{3.5}$$

where $a_T = \frac{1}{4}(d+c)^2 d^{-1}$.

For purposes of this work, we will consider a more general form of (3.4) which includes generic expressions of the reaction terms of the partial differential equations. More precisely, we will consider

$$\begin{aligned}
\tau_u \frac{\partial^2 u(x,t)}{\partial t^2} + \frac{\partial u(x,t)}{\partial t} &= \frac{\partial F(u(x,t),v(x,t))}{\partial u} + d_u \nabla^{\alpha_1} u(x,t), \quad \forall (x,t) \in \Omega, \\
\tau_v \frac{\partial^2 v(x,t)}{\partial t^2} + \frac{\partial v(x,t)}{\partial t} &= \frac{\partial G(u(x,t),v(x,t))}{\partial v} + d_v \nabla^{\alpha_2} v(x,t), \quad \forall (x,t) \in \Omega, \\
\text{such that } &\begin{cases} u(x,0) = \phi^u(x), & \forall x \in B, \\ v(x,0) = \phi^v(x), & \forall x \in B. \\ \dfrac{\partial u}{\partial t}(x,0) = \psi^u(x), & \forall x \in B, \\ \dfrac{\partial v}{\partial t}(x,0) = \psi^v(x), & \forall x \in B, \end{cases}
\end{aligned} \tag{3.6}$$

where $F, G : \mathbb{R}^2 \to \mathbb{R}$ are sufficiently smooth functions. Note that the model (3.4) is a particular form of (3.6) with

$$F(u,v) = \tfrac{1}{2}u^2 - auv + \tfrac{1}{2}bu^2 v - \tfrac{1}{4}u^4, \quad \forall u, v \in \mathbb{R}, \tag{3.7}$$

$$G(u,v) = uv - \tfrac{1}{2}cv^2, \quad \forall u, v \in \mathbb{R}. \tag{3.8}$$

In this work, we follow a finite-difference approach to approximate the solutions of (3.6), and use fractional centered differences to estimate Riesz space-fractional derivatives in a consistent form [94].

Definition 3.2.3. For any function $f : \mathbb{R} \to \mathbb{R}$, any $h > 0$ and $\beta > -1$, the *fractional centered difference* of order β of f at the point x is defined as

$$\Delta_h^{(\beta)} f(x) = \sum_{k=-\infty}^{\infty} g_k^{(\beta)} f(x - kh), \quad \forall x \in \mathbb{R}, \tag{3.9}$$

where

$$g_k^{(\beta)} = \frac{(-1)^k \Gamma(\beta+1)}{\Gamma(\frac{\beta}{2} - k + 1)\Gamma(\frac{\beta}{2} + k + 1)}, \quad \forall k \in \mathbb{Z}. \tag{3.10}$$

Lemma 3.2.4 (Wang *et al.* [133])**.** *If $0 < \beta \leq 2$ and $\beta \neq 1$ then the coefficients $(g_k^{(\beta)})_{k=-\infty}^{\infty}$ satisfy:*

(a) $g_0^{(\beta)} > 0$,

(b) $g_k^{(\beta)} = g_{-k}^{(\beta)} \leq 0$ *for all* $k \neq 0$, *and*

(c) $\displaystyle\sum_{k=-\infty}^{\infty} g_k^{(\beta)} = 0$. *As a consequence, it follows that* $\displaystyle g_0^{(\beta)} = -\sum_{\substack{k=-\infty \\ k\neq 0}}^{\infty} g_k^{(\beta)}$.

Lemma 3.2.5 (Wang *et al.* [133])**.** *Let $f \in \mathcal{C}^5(\mathbb{R})$ and assume that all its derivatives up to order five are integrable. If $0 < \beta \leq 2$ and $\beta \neq 1$ then, for almost all x,*

$$-\frac{\Delta_h^{\beta} f(x)}{h^{\beta}} = \frac{d^{\beta} f(x)}{d|x|^{\beta}} + \mathcal{O}(h^2). \tag{3.11}$$

3.3 Numerical methodology

In this section, we introduce the discrete nomenclature and the numerical method to approximate the solutions of (3.4). The notation will be similar to that employed in [80]. We describe it here briefly for the sake of convenience.

Let $I_q = \{1, \ldots, q\}$ and $\overline{I}_q = I_q \cup \{0\}$, for each $q \in \mathbb{N}$. Let $K, M, N \in \mathbb{N}$, and define the spatial partition norms $h_1 = (b_1 - a_1)/M$ and $h_2 = (b_2 - a_2)/N$ in the x_1- and the x_2-directions, respectively. We will consider the following uniform partitions of the intervals $[a_1, b_1]$ and $[a_2, b_2]$, respectively:

$$a_1 = x_{1,0} < x_{1,1} < \ldots < x_{1,m} < \ldots < x_{1,M} = b_1, \quad \forall m \in \overline{I}_M, \tag{3.12}$$

$$a_2 = x_{2,0} < x_{2,1} < \ldots < x_{2,n} < \ldots < x_{2,N} = b_2, \quad \forall n \in \overline{I}_N. \tag{3.13}$$

Let $J = I_{M-1} \times I_{N-1}$ and $\overline{J} = \overline{I}_M \times \overline{I}_N$. We will fix a uniform partition of $[0,T]$ consisting of K subintervals, namely,

$$0 = t_0 < t_1 < \ldots < t_k < \ldots < t_K = T, \quad \forall k \in \overline{I}_K, \tag{3.14}$$

and define $\tau = T/K$. For each $(m,n,k) \in \overline{J} \times \overline{I}_K$, let $\mathbf{u}_{m,n}^k$ and $\mathbf{v}_{m,n}^k$ represent approximations to the exact values of the solutions u and v of (3.6), respectively, at the point $x_{m,n} = (x_{1,m}, x_{2,n})$ and time t_k. Let $\varphi_{m,n} = \varphi(x_{m,n})$ for any function $\varphi : \overline{B} \to \mathbb{R}$ and $(m,n) \in \overline{J}$.

Let $h = (h_1, h_2)$ and $h_* = h_1 h_2$. Convey that $R_h = \{x_j\}_{j \in \overline{J}} \subseteq \mathbb{R}^2$ and let $\mathcal{V}_h$ be the real vector space of all real functions on R_h. For any $\mathbf{u} \in \mathcal{V}_h$ and $j \in \overline{J}$, let $\mathbf{u}_j = \mathbf{u}(x_j)$. We represent any numerical approximation to the solution of (3.6) by $(\mathbf{u}, \mathbf{v})$, where $\mathbf{u} = (\mathbf{u}^k)_{k=0}^K$ and $\mathbf{v} = (\mathbf{v}^k)_{k=0}^K$, and $\mathbf{u}^k = (\mathbf{u}_j^k)_{j \in \overline{J}}$ and $\mathbf{v}^k = (\mathbf{v}_j^k)_{j \in \overline{J}}$, for each $k \in \overline{I}_N$. Alternatively, we will employ the nomenclature $(\mathbf{u}, \mathbf{v}) = ((\mathbf{u}^k, \mathbf{v}^k))_{k=0}^K$. In the following and unless we say otherwise, we will use w to represent u or v. Likewise, $\mathbf{w}$ will denote $\mathbf{u}$ or $\mathbf{v}$.

Definition 3.3.1. Define 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

$$\langle \mathbf{u}, \mathbf{v} \rangle = h_* \sum_{j \in \overline{J}} \mathbf{u}_j \mathbf{v}_j, \quad \|\mathbf{u}\|_1 = h_* \sum_{j \in \overline{J}} |\mathbf{u}_j|, \quad \forall \mathbf{u}, \mathbf{v} \in \mathcal{V}_h. \tag{3.15}$$

The Euclidean norm induced by $\langle \cdot, \cdot \rangle$ will be denoted by $\| \cdot \|_2$, and $\| \cdot \|_\infty$ will be the usual infinity norm in $\mathcal{V}_h$.

Definition 3.3.2. For each sequence $(\mathbf{w}^k)_{k=0}^K \subseteq \mathcal{V}_h$, $(m,n) \in \overline{J}$ and $k \in I_{K-1}$, define the following linear operators:

$$\delta_t^{(1)} \mathbf{w}_{m,n}^k = \frac{\mathbf{w}_{m,n}^{k+1} - \mathbf{w}_{m,n}^{k-1}}{2\tau}, \tag{3.16}$$

$$\delta_t^{(2)} \mathbf{w}_{m,n}^k = \frac{\mathbf{w}_{m,n}^{k+1} - 2\mathbf{w}_{m,n}^k + \mathbf{w}_{m,n}^{k-1}}{\tau^2}, \tag{3.17}$$

$$\mu_t \mathbf{w}_{m,n}^k = \frac{\mathbf{w}_{m,n}^{k+1} + \mathbf{w}_{m,n}^k}{2}, \tag{3.18}$$

$$\mu_t^{(1)} \mathbf{w}_{m,n}^k = \frac{\mathbf{w}_{m,n}^{k+1} + \mathbf{w}_{m,n}^{k-1}}{2}. \tag{3.19}$$

Obviously, the operator (3.16) provides a consistent approximation of the first-order partial derivative of w with respect to t at $(x_{m,n}, t_k)$, while (3.17) approximates consistently the second-order partial derivative of w with respect to t, and (3.18) and (3.19) estimate consistently the value of w at that point.

Definition 3.3.3. Let $0 < \beta \leq 2$ with $\beta \neq 1$. For each $(\mathbf{w}^k)_{k=0}^K \subseteq \mathcal{V}_h$, $(m,n) \in \overline{J}$ and $k \in \overline{I}_K$, define the linear operators

$$\delta_{x_1}^{(\beta)} \mathbf{w}_{m,n}^k = -\frac{1}{h_1^\beta} \sum_{j=0}^{M} g_{m-j}^{(\beta)} \mathbf{w}_{j,n}^k, \quad \delta_{x_2}^{(\beta)} \mathbf{w}_{m,n}^k = -\frac{1}{h_2^\beta} \sum_{j=0}^{N} g_{n-j}^{(\beta)} \mathbf{w}_{m,j}^k. \tag{3.20}$$

In light of Lemma 3.2.5, the operators in Definition 3.3.3 yield second-order approximations of the fractional derivatives of w of order β with respect to x_1 and x_2, respectively, at the point $(x_{m,n}, t_k)$, for each $(m,n,k) \in \overline{J} \times \overline{I}_K$. So,

$$\delta_x^{(\beta)} \mathbf{w}_{m,n}^k = \delta_{x_1}^{(\beta)} \mathbf{w}_{m,n}^k + \delta_{x_2}^{(\beta)} \mathbf{w}_{m,n}^k, \quad \forall (m,n,k) \in \overline{J} \times \overline{I}_K, \tag{3.21}$$

is a second-order approximation of the fractional Laplacian of w of order β at $(x_{m,n}, t_k)$.

Definition 3.3.4. For each $(\mathbf{u}^k)_{k=0}^K, (\mathbf{v}^k)_{k=0}^K, (\mathbf{w}^k)_{k=0}^K \subseteq \mathcal{V}_h$, and each $j \in \overline{J}$ and $k \in I_{K-1}$, define the

nonlinear operators

$$\delta_{u,t}^{(1)}F_j^k(\mathbf{w},\mathbf{v}) = \begin{cases} \dfrac{F(\mathbf{w}_j^{k+1},\mathbf{v}_j^k)-F(\mathbf{u}_j^{k-1},\mathbf{v}_j^k)}{\mathbf{w}_j^{k+1}-\mathbf{u}_j^{k-1}}, & \text{if } \mathbf{w}_j^{k+1}\neq\mathbf{u}_j^{k-1}, \\ \dfrac{\partial F(\mathbf{u}_j^k,\mathbf{v}_j^k)}{\partial u}, & \text{if } \mathbf{w}_j^{k+1}=\mathbf{u}_j^{k-1}, \end{cases} \tag{3.22}$$

$$\delta_{v,t}^{(1)}G_j^k(\mathbf{u},\mathbf{w}) = \begin{cases} \dfrac{G(\mathbf{u}_j^k,\mathbf{w}_j^{k+1})-G(\mathbf{u}_j^k,\mathbf{v}_j^{k-1})}{\mathbf{w}_j^{k+1}-\mathbf{v}_j^{k-1}}, & \text{if } \mathbf{w}_j^{k+1}\neq\mathbf{v}_j^{k-1}, \\ \dfrac{\partial G(\mathbf{u}_j^k,\mathbf{v}_j^k)}{\partial v}, & \text{if } \mathbf{w}_j^{k+1}=\mathbf{v}_j^{k-1}. \end{cases} \tag{3.23}$$

Note that $\delta_{u,t}^{(1)}F^k(\mathbf{w},\mathbf{v}) = (\delta_{u,t}^{(1)}F_j^k(\mathbf{w},\mathbf{v}))_{j\in\overline{J}}$ and $\delta_{v,t}^{(1)}G^k(\mathbf{u},\mathbf{w}) = (\delta_{v,t}^{(1)}G_j^k(\mathbf{u},\mathbf{w}))_{j\in\overline{J}}$ are both continuous operators on $\mathcal{V}_h$ for each $k\in I_{K-1}$, whenever F and G are differentiable on $\mathbb{R}^2$.

For each $P\in\mathbb{N}$ and $\beta\in(0,1)\cup(1,2]$, define the real matrix A_P of size $(P+1)\times(P+1)$ by

$$A_P^{(\beta)} = \begin{pmatrix} g_0^{(\beta)} & g_1^{(\beta)} & \cdots & g_P^{(\beta)} \\ g_1^{(\beta)} & g_0^{(\beta)} & \cdots & g_{P-1}^{(\beta)} \\ \vdots & \vdots & \ddots & \vdots \\ g_P^{(\beta)} & g_{P-1}^{(\beta)} & \cdots & g_0^{(\beta)} \end{pmatrix}. \tag{3.24}$$

We define the diagonal block-matrices $A_{x_1}^{(\beta)}$ and $A_{x_2}^{(\beta)}$ of sizes of sizes $[(M+1)\times(N+1)]\times[(M+1)\times(N+1)]$ using direct sums of matrices:

$$A_{x_1}^{(\beta)} = \underbrace{A_M^{(\beta)}\oplus A_M^{(\beta)}\oplus\cdots\oplus A_M^{(\beta)}}_{(N+1)\text{-times}}, \qquad A_{x_2}^{(\beta)} = \underbrace{A_N^{(\beta)}\oplus A_N^{(\beta)}\oplus\cdots\oplus A_N^{(\beta)}}_{(M+1)\text{-times}}. \tag{3.25}$$

Lemma 3.3.5 (Macías-Díaz [79])**.** *The following are properties satisfied by $A_{x_i}^{(\beta)}$, for each $\beta\in(0,1)\cup(1,2]$ and $i\in I_2$:*

(a) *$A_{x_i}^{(\beta)}$ is real and symmetric, so Hermitian.*

(b) *$A_{x_i}^{(\beta)}$ is strictly diagonally dominant,*

(c) *All the eigenvalues of $A_{x_i}^{(\beta)}$ are positive real numbers bounded from above by $2g_0^{(\beta)}$.*

(d) *$A_{x_i}^{(\beta)}$ is positive-definite.*

Proof. The proof is similar to that in [79, Lemma 4.2]. □

Note that any $\mathbf{u}\in\mathcal{V}_h$ may be represented in vector form alternatively as

$$\mathbf{u}_{x_1} = (\underbrace{\mathbf{u}_{0,0},\mathbf{u}_{1,0},\ldots,\mathbf{u}_{M,0}}, \underbrace{\mathbf{u}_{0,1},\mathbf{u}_{1,1},\ldots,\mathbf{u}_{M,1}}, \ldots, \underbrace{\mathbf{u}_{0,N},\mathbf{u}_{1,N},\ldots,\mathbf{u}_{M,N}}), \tag{3.26}$$

$$\mathbf{u}_{x_2} = (\underbrace{\mathbf{u}_{0,0},\mathbf{u}_{0,1},\ldots,\mathbf{u}_{0,N}}, \underbrace{\mathbf{u}_{1,0},\mathbf{u}_{1,1},\ldots,\mathbf{u}_{1,N}}, \ldots, \underbrace{\mathbf{u}_{M,0},\mathbf{u}_{M,1},\ldots,\mathbf{u}_{M,N}}). \tag{3.27}$$

It is straightforward to see then that $\delta_{x_i}^{(\beta)}\mathbf{u} = -h_i^{-\beta}A_{x_i}^{(\beta)}\mathbf{u}_{x_i}^\top$ and $\langle\mathbf{u},-\delta_{x_i}^{(\beta)}\mathbf{v}\rangle = h_*h_i^{-\beta}\mathbf{u}_{x_i}A_{x_i}^{(\beta)}\mathbf{v}_{x_i}^\top$, for each $i\in I_2$, each $\beta\in(0,1)\cup(1,2]$ and $\mathbf{u},\mathbf{v}\in\mathcal{V}_h$. These facts will be used in the proof of the next Lemma.

Lemma 3.3.6. *For each $i\in I_2$ and $\beta\in(0,1)\cup(1,2]$, there exists a unique positive self-adjoint (square-root) operator $\Lambda_{x_i}^{(\beta)}:\mathcal{V}_h\to\mathcal{V}_h$, such that $\langle-\delta_{x_i}^{(\beta)}\mathbf{u},\mathbf{v}\rangle = \langle\Lambda_{x_i}^{(\beta)}\mathbf{u},\Lambda_{x_i}^{(\beta)}\mathbf{v}\rangle$, for each $\mathbf{u},\mathbf{v}\in\mathcal{V}_h$.*

Proof. Recall that $A_{x_i}^{(\beta)}$ is a symmetric matrix, and note that $-\delta_{x_i}^{(\beta)}:\mathcal{V}_h\to\mathcal{V}_h$ is a linear operator that satisfies the following identities for each $u,v\in\mathcal{V}_h$:

$$\left\langle\mathbf{u},-\delta_{x_i}^{(\beta)}\mathbf{v}\right\rangle = h_*h_i^{-\beta}\mathbf{u}_{x_i}A_{x_i}^{(\beta)}\mathbf{v}_{x_i}^\top = h_*h_i^{-\beta}\left(\mathbf{u}_{x_i}A_{x_i}^{(\beta)}\mathbf{v}_{x_i}^\top\right)^\top = h_*h_i^{-\beta}\mathbf{v}_{x_i}A_{x_i}^{(\beta)}\mathbf{u}_{x_i}^\top = \left\langle-\delta_{x_i}^{(\beta)}\mathbf{u},\mathbf{v}\right\rangle. \tag{3.28}$$

This means that $-\delta_{x_i}^{(\beta)}$ is a self-adjoint operator on the Hilbert space $\mathcal{V}_h$. Moreover, the fact that the matrix $A_{x_i}^{(\beta)}$ is positive-definite implies that $\left\langle \mathbf{u}, -\delta_{x_i}^{(\beta)}\mathbf{u} \right\rangle = h_* h_i^{-\beta} \mathbf{u}_{x_i} A_{x_i}^{(\beta)} \mathbf{u}_{x_i}^\top \geq 0$ for each $\mathbf{u} \in \mathcal{V}$. It follows that $-\delta_{x_i}^{(\beta)}$ has a unique square-root operator $\Lambda_{x_i}^{(\beta)}$, which has the desired properties. □

For each $\beta \in (0,1) \cup (1,2]$, define

$$g_h^{(\beta)} = 2h_* g_0^{(\beta)} \sqrt{h_1^{-2\beta} + h_2^{-2\beta}}, \qquad \gamma_h^{(\beta)} = 2h_* g_0^{(\beta)} \left(h_1^{-\beta} + h_2^{-\beta} \right) \tag{3.29}$$

Using this nomenclature, the following result summarizes some easy properties of the fractional centered difference operators and their respective square-roots. Those properties will be used for the remainder of this chapter.

Lemma 3.3.7. *Let $\mathbf{v} \in \mathcal{V}_h$ and $i \in I_2$. If $\beta \in (0,1) \cup (1,2]$ then*

(a) $\|\Lambda_{x_i}^{(\beta)} \mathbf{v}\|_2^2 \leq 2g_0^{(\beta)} h_* h_i^{-\beta} \|\mathbf{v}\|_2^2$,

(b) $\|\delta_{x_i}^{(\beta)} \mathbf{v}\|_2^2 = \|\Lambda_{x_i}^{(\beta)} \Lambda_{x_i}^{(\beta)} \mathbf{v}\|_2^2$,

(c) $\|\delta_{x_i}^{(\beta)} \mathbf{v}\|_2^2 \leq 4 \left(g_0^{(\beta)} h_* h_i^{-\beta} \right)^2 \|\mathbf{v}\|_2^2$ *and*

(d) $\displaystyle\sum_{i \in I_2} \|\delta_{x_i}^{(\beta)} \mathbf{v}\|_2^2 \leq \left(g_h^{(\beta)} \|\mathbf{v}\|_2 \right)^2$ *and* $\displaystyle\sum_{i \in I_2} \|\Lambda_{x_i}^{(\beta)} \mathbf{v}\|_2^2 \leq \gamma_h^{(\beta)} \|\mathbf{v}\|_2^2$.

Proof.

(a) The properties of matrix $A_{x_i}^{(\beta)}$ summarized in Lemma 3.3.5 guarantee $\mathbf{v}_{x_i} A_{x_i}^{(\beta)} \mathbf{v}_{x_i}^\top \leq 2g_0^{(\beta)} \|\mathbf{v}_{x_i}\|_2^2$ holds. The remarks before the proof of Lemma 3.3.6 lead to $\|\Lambda_{x_i}^{(\beta)} \mathbf{v}\|_2^2 = h_* h_i^{-\beta} \mathbf{v}_{x_i} A_{x_i}^{(\beta)} \mathbf{v}_{x_i}^\top \leq 2g_0^{(\beta)} h_* h_i^{-\beta} \|\mathbf{v}\|_2^2$.

(b) Using Lemma 3.3.6, we obtain

$$\|\delta_{x_i}^{(\beta)} \mathbf{v}\|_2^2 = \langle -\delta_{x_i}^{(\beta)} \mathbf{v}, -\delta_{x_i}^{(\beta)} \mathbf{v} \rangle = \langle \Lambda_{x_i}^{(\beta)} \mathbf{v}, -\delta_{x_i}^{(\beta)} \Lambda_{x_i}^{(\beta)} \mathbf{v} \rangle = \langle \Lambda_{x_i}^{(\beta)} \Lambda_{x_i}^{(\beta)} \mathbf{v}, \Lambda_{x_i}^{(\beta)} \Lambda_{x_i}^{(\beta)} \mathbf{v} \rangle = \|\Lambda_{x_i}^{(\beta)} \Lambda_{x_i}^{(\beta)} \mathbf{v}\|_2^2. \tag{3.30}$$

(c) This property is a consequence of (a) and (b). Indeed, note that

$$\|\delta_{x_i}^{(\beta)} \mathbf{v}\|_2^2 = \|\Lambda_{x_i}^{(\beta)} \Lambda_{x_i}^{(\beta)} \mathbf{v}\|_2^2 \leq 2g_0^{(\beta)} h_* h_i^{-\beta} \|\Lambda_{x_i}^{(\beta)} \mathbf{v}\|_2^2 \leq 4 \left(g_0^{(\beta)} h_* h_i^{-\beta} \right)^2 \|\mathbf{v}\|_2^2. \tag{3.31}$$

(d) This property follows immediately from (c). □

Assume that ψ^u and ψ^v represent the exact values of the solutions u and v, respectively, at the time t_1. Under these circumstances, the numerical method to approximate the solutions of (3.6) is described by the following scheme:

$$\begin{aligned} \tau_u \delta_t^{(2)} \mathbf{u}_j^k + \delta_t^{(1)} \mathbf{u}_j^k &= \delta_{u,t}^{(1)} F_j^k(\mathbf{u}, \mathbf{v}) + d_u \delta_x^{(\alpha_1)} \mathbf{u}_j^k, \quad \forall (j,k) \in \overline{J} \times I_{K-1}, \\ \tau_v \delta_t^{(2)} \mathbf{v}_j^k + \delta_t^{(1)} \mathbf{v}_j^k &= \delta_{v,t}^{(1)} G_j^k(\mathbf{u}, \mathbf{v}) + d_v \delta_x^{(\alpha_2)} \mathbf{v}_j^k, \quad \forall (j,k) \in \overline{J} \times I_{K-1}, \\ \text{such that } & \begin{cases} \mathbf{u}_j^0 = \phi^u(x_j), & \forall j \in \overline{J}, \\ \mathbf{v}_j^0 = \phi^v(x_j), & \forall j \in \overline{J}, \\ \mathbf{u}_j^1 = \psi^u(x_j), & \forall j \in \overline{J}, \\ \mathbf{v}_j^1 = \psi^v(x_j), & \forall j \in \overline{J}. \end{cases} \end{aligned} \tag{3.32}$$

The method is an explicit scheme, in the sense that the solutions $\mathbf{u}_j^{k+1}$ and $\mathbf{v}_j^{k+1}$ of the discrete system at the kth iteration are obtained separately by solving two polynomial equations that depend exclusively on $\mathbf{u}_j^{k+1}$ and $\mathbf{v}_j^{k+1}$, respectively. The finite-difference scheme will be coded in Fortran using an implementation of the Newton–Raphson method for solving nonlinear equations. For the simulations in Section 3.5, we will use a maximum number of iterations equal to 20 and a tolerance in the infinity norm of 1×10^{-8} as stopping criteria.

Lemma 3.3.8 (Brouwer's fixed-point theorem [2])**.** *Let $\mathcal{V}$ be a finite-dimensional vector space over $\mathbb{R}$, and $\langle\cdot,\cdot\rangle$ an inner product on $\mathcal{V}$. Suppose that $f:\mathcal{V}\to\mathcal{V}$ is continuous, and that there exists $\lambda>0$ such that $\langle f(\mathbf{w}),\mathbf{w}\rangle\geq 0$, for each $\mathbf{w}\in\mathcal{V}$ with $\|\mathbf{w}\|=\lambda$. Then there exists $\mathbf{w}\in\mathcal{V}$ with $\|\mathbf{w}\|\leq\lambda$, satisfying $f(\mathbf{w})=0$.* □

Theorem 3.3.9 (Existence of solutions)**.** *Let F and G be differentiable in the first and second arguments, respectively, and assume that those derivatives are bounded. Then* (3.32) *has a solution for any set of initial conditions.*

Proof. We prove this result using induction. Notice that the approximations $(\mathbf{u}^0,\mathbf{v}^0)$ and $(\mathbf{u}^1,\mathbf{v}^1)$ exist, so assume that $(\mathbf{u}^{k-1},\mathbf{v}^{k-1})$ and $(\mathbf{u}^k,\mathbf{v}^k)$ have been obtained for some $k\in I_{K-1}$. Note that the continuity of the operator $\delta^{(1)}_{u,t}F^k$, together with the boundedness of the first derivative of F imply that $\delta^{(1)}_{u,t}F^k$ is bounded. Let $h^u:\mathcal{V}_h\to\mathcal{V}_h$ be the continuous function whose jth component $h^u_j:\mathcal{V}_h\to\mathbb{R}$ is given by

$$h^u_j(\mathbf{w})=\tau_u\frac{\mathbf{w}_j-2\mathbf{u}^k_j+\mathbf{u}^{k-1}_j}{\tau^2}+\frac{\mathbf{w}_j-\mathbf{u}^{k-1}_j}{2\tau}-\delta^{(1)}_{u,t}F^k_j(\mathbf{w},\mathbf{v})-\delta^{(\alpha_1)}_x\mathbf{u}^k_j,\quad\forall\mathbf{w}\in\mathcal{V}_h,\forall j\in\overline{J}.\tag{3.33}$$

Using the boundedness of $\delta^{(1)}_{u,t}F^k$ and the Cauchy–Schwarz inequality, and applying then the properties of Lemma 3.3.7, there exists a constant $K_1\in\mathbb{R}^+$ such that

$$\begin{aligned}\langle h(\mathbf{w}),\mathbf{w}\rangle\geq{}&\frac{\tau_u}{\tau}\|\mathbf{w}\|_2\left(\|\mathbf{w}\|_2-2\|\mathbf{u}^k\|_2-\|\mathbf{u}^{k-1}\|_2\right)\\&+\frac{1}{2\tau}\|\mathbf{w}\|_2\left(\|\mathbf{w}\|_2-\|\mathbf{u}^{k-1}\|_2\right)-K_1\|\mathbf{w}\|_2-\|\delta^{(\alpha_1)}_x\mathbf{u}^k\|_2\|\mathbf{w}\|_2,\end{aligned}\tag{3.34}$$

for all $\mathbf{w}\in\mathcal{V}_h$. After regrouping, it follows that $\langle h(\mathbf{w}),\mathbf{w}\rangle\geq c_1\|\mathbf{w}\|_2(\|\mathbf{w}\|_2-\lambda_1)$ for each $\mathbf{w}\in\mathcal{V}_h$. Here,

$$c_1=\frac{2\tau_u+\tau}{2\tau^2},\tag{3.35}$$

$$\lambda_1=\frac{(4\tau_u+2\tau^2g^{(\alpha_1)}_h)\|\mathbf{u}^k\|_2+(2\tau_u+\tau)\|\mathbf{u}^{k-1}\|_2+2\tau^2K_1}{2\tau_u+\tau}.\tag{3.36}$$

It is obvious that both c_1 and λ_1 are positive, and that $\langle f(\mathbf{w}),\mathbf{w}\rangle\geq 0$ for each $\mathbf{w}\in\mathcal{V}_h$ with $\|\mathbf{w}\|_2=\lambda_1$. By Brouwer's fixed-point theorem, there exists $\mathbf{u}^{k+1}\in\mathcal{V}_h$ with $\|\mathbf{u}^{k+1}\|_2\leq\lambda_1$, such that $h^u(\mathbf{u}^{k+1})=0$. In similar fashion, there exist $\lambda_2>0$ and $\mathbf{v}^{k+1}\in\mathcal{V}_h$ with $\|\mathbf{v}^{k+1}\|_2\leq\lambda_2$, such that $h^v(\mathbf{v}^{k+1})=0$. It follows that there exists a solution $(\mathbf{u}^{k+1},\mathbf{v}^{k+1})$ of the method at the kth temporal step, and the conclusion follows now by induction. □

3.4 Numerical properties

The purpose of this section is to establish the most important numerical properties of the method (3.32). More concretely, we will prove that the method is a quadratically consistent technique which is both stable and quadratically convergent. Moreover, we will prove the existence and the uniqueness of the solutions of our numerical method as a corollary of Theorem 3.3.9 and the numerical stability.

To establish the consistency property of the method, we define the continuous operators

$$\mathcal{L}_u(u(x,t),v(x,t))=\tau_u\frac{\partial^2u(x,t)}{\partial t^2}+\frac{\partial u(x,t)}{\partial t}-\frac{\partial F(u(x,t),v(x,t))}{\partial u}-d_u\nabla^{\alpha_1}u(x,t),\quad\forall(x,t)\in\Omega,\tag{3.37}$$

$$\mathcal{L}_v(u(x,t),v(x,t))=\tau_v\frac{\partial^2v(x,t)}{\partial t^2}+\frac{\partial v(x,t)}{\partial t}-\frac{\partial G(u(x,t),v(x,t))}{\partial v}-d_v\nabla^{\alpha_2}v(x,t),\quad\forall(x,t)\in\Omega.\tag{3.38}$$

We also define the following discrete operators:

$$\mathbf{L}_u(\mathbf{u}^k_j,\mathbf{v}^k_j)=\tau_u\delta^{(2)}_t\mathbf{u}^k_j+\delta^{(1)}_t\mathbf{u}^k_j-\delta^{(1)}_{u,t}F^k_j(\mathbf{u},\mathbf{v})-d_u\delta^{(\alpha_1)}_x\mathbf{u}^k_j,\quad\forall(j,k)\in\overline{J}\times I_{K-1},\tag{3.39}$$

$$\mathbf{L}_v(\mathbf{u}^k_j,\mathbf{v}^k_j)=\tau_v\delta^{(2)}_t\mathbf{v}^k_j+\delta^{(1)}_t\mathbf{v}^k_j-\delta^{(1)}_{v,t}G^k_j(\mathbf{u},\mathbf{v})-d_v\delta^{(\alpha_2)}_x\mathbf{v}^k_j,\quad\forall(j,k)\in\overline{J}\times I_{K-1}.\tag{3.40}$$

Moreover, we let $\mathcal{L}(x_j,t_k)=(\mathcal{L}_u(u(x_j,t_k),v(x_j,t_k)),\mathcal{L}_v(u(x_j,t_k),v(x_j,t_k)))$, for each $(j,k)\in\overline{J}\times I_{K-1}$. Also, let us define $\mathbf{L}^k_j=(\mathbf{L}_u(\mathbf{u}^k_j,\mathbf{v}^k_j),\mathbf{L}_v(\mathbf{u}^k_j,\mathbf{v}^k_j))$, for each $(j,k)\in\overline{J}\times I_{K-1}$. We will convey in the following that $u^k_j=u(x_j,t_k)$ and $v^k_j=v(x_j,t_k)$, for each $(j,k)\in\overline{J}\times\overline{I}_K$.

Theorem 3.4.1 (Consistency). *If $u, v \in \mathcal{C}^5(\overline{\Omega})$ then there exists a constant $C \in \mathbb{R}^+$ independent of τ and h, such that*

$$\|\mathcal{L}(x_j, t_k) - \mathbf{L}_j^k\|_\infty \leq C(\tau^2 + \|h\|_2^2), \quad \forall (j,k) \in \overline{J} \times I_{K-1}. \tag{3.41}$$

Proof. We will employ here the usual argument with Taylor polynomials and Lemma 3.2.5. Using the smoothness of the functions u and v, there exist constants $C_1^w, C_2^w \in \mathbb{R}^+$ for $w = u, v$, such that

$$\left|\delta_t^{(2)} w_j^k - \frac{\partial^2 w(x_j,t_k)}{\partial t^2}\right| \leq C_1^w \tau^2, \quad \forall (j,k) \in \overline{J} \times I_{K-1}, \tag{3.42}$$

$$\left|\delta_t^{(1)} w_j^k - \frac{\partial w(x_j,t_k)}{\partial t}\right| \leq C_2^w \tau^2, \quad \forall (j,k) \in \overline{J} \times I_{K-1}. \tag{3.43}$$

Similarly, there exist constants $C_3^w, C_4^w \in \mathbb{R}^+$ for $w = u, v$, with the properties

$$\begin{aligned}
\left|\delta_{u,t}^{(1)} F_j^k(\mathbf{u}_j^k, \mathbf{v}_j^k) - \frac{\partial F(u(x_j,t_k), v(x_j,t_k))}{\partial u}\right| &\leq C_3^u \tau^2, \quad \forall (j,k) \in \overline{J} \times I_{K-1}, \\
\left|\delta_{v,t}^{(1)} G_j^k(\mathbf{u}_j^k, \mathbf{v}_j^k) - \frac{\partial G(u(x_j,t_k), v(x_j,t_k))}{\partial v}\right| &\leq C_3^v \tau^2, \quad \forall (j,k) \in \overline{J} \times I_{K-1}, \\
\left|\delta_x^{(\alpha_1)} \mathbf{u}_j^k - \nabla^{\alpha_1} u(x_j,t_k)\right| &\leq C_4^u \|h\|_2^2, \quad \forall (j,k) \in \overline{J} \times I_{K-1}, \\
\left|\delta_x^{(\alpha_2)} \mathbf{v}_j^k - \nabla^{\alpha_2} v(x_j,t_k)\right| &\leq C_4^v \|h\|_2^2, \quad \forall (j,k) \in \overline{J} \times I_{K-1}.
\end{aligned} \tag{3.44}$$

Let $C^w = \max\{\tau_w C_1^w, C_2^w, C_3^w, d_w C_4^w\}$ for each $w = u, v$. Then the conclusion of the theorem readily follows from the triangle inequality, letting $C = C^u \vee C^v$. □

We will require the following lemmas.

Lemma 3.4.2 (Pen-Yu [95]). *Let $(\omega^k)_{k=0}^K$ and $(\rho^k)_{k=0}^K$ be sequences of nonnegative numbers, and let $C \geq 0$ be such that*

$$\omega^k \leq \rho^k + C\tau \sum_{l=0}^{k-1} \omega^l, \quad \forall k \in \overline{I}_K. \tag{3.45}$$

Then $\omega^k \leq \rho^k e^{Ck\tau}$ for each $k \in \overline{I}_K$. □

Lemma 3.4.3. *Let $F, G \in \mathcal{C}^2(\mathbb{R}^2)$ have partial derivatives of the second order with respect to u and v, respectively, which are bounded in $\mathbb{R}^2$. Let $(\mathbf{u}, \mathbf{v})$ and $(\tilde{\mathbf{u}}, \tilde{\mathbf{v}})$ be solutions of (3.32), and let $\mathbf{e}^{u,k} = \mathbf{u}^k - \tilde{\mathbf{u}}^k$ and $\mathbf{e}^{v,k} = \mathbf{v}^k - \tilde{\mathbf{v}}^k$ for each $k \in \overline{I}_K$. Let $(\mathbf{R}^{u,k})_{k=0}^K, (\mathbf{R}^{v,k})_{k=0}^K \subseteq \mathcal{V}_h$, and let $\widetilde{F}^k = \delta_{u,t}^{(1)} F^k(\mathbf{u}^k, \mathbf{v}^k) - \delta_{u,t}^{(1)} F^k(\tilde{\mathbf{u}}^k, \tilde{\mathbf{v}}^k)$ and $\widetilde{G}^k = \delta_{v,t}^{(1)} G^k(\mathbf{u}^k, \mathbf{v}^k) - \delta_{v,t}^{(1)} G^k(\tilde{\mathbf{u}}^k, \tilde{\mathbf{v}}^k)$ for each $k \in I_k$. Then there exist constants $C_1^u, C_1^v \in \mathbb{R}^+$ which depend only on F and G, respectively, such that*

$$\left|\langle 2\widetilde{F}^k, \delta_t^{(1)} \mathbf{e}^{u,k} \rangle\right| \leq C_1^u \left(\|\delta_t \mathbf{e}^{u,k}\|_2^2 + \|\delta_t \mathbf{e}^{u,k-1}\|_2^2 + \|\mathbf{e}^{u,k+1}\|_2^2 + \|\mathbf{e}^{u,k-1}\|_2^2\right), \quad \forall k \in I_{K-1}, \tag{3.46}$$

$$\left|\langle 2\widetilde{G}^k, \delta_t^{(1)} \mathbf{e}^{v,k} \rangle\right| \leq C_1^v \left(\|\delta_t \mathbf{e}^{v,k}\|_2^2 + \|\delta_t \mathbf{e}^{v,k-1}\|_2^2 + \|\mathbf{e}^{v,k+1}\|_2^2 + \|\mathbf{e}^{v,k-1}\|_2^2\right), \quad \forall k \in I_{K-1}. \tag{3.47}$$

Moreover, there exist constants $C_2^u, C_3^u \in \mathbb{R}^+$ that depend only on F as well as constants $C_2^v, C_3^v \in \mathbb{R}^+$ that depend only on G, such that

$$2\tau \left|\sum_{l=1}^k \langle \mathbf{R}^{u,l} - \widetilde{F}^l, \delta_t^{(1)} \mathbf{e}^{u,l} \rangle\right| \leq 2\tau \sum_{l=0}^k \|\mathbf{R}^{u,l}\|_2^2 + C_2^u \|\mathbf{e}^{u,0}\|_2^2 + C_3^u \tau \sum_{l=0}^k \|\delta_t \mathbf{e}^{u,l}\|_2^2, \quad \forall k \in I_{N-1}, \tag{3.48}$$

$$2\tau \left|\sum_{l=1}^k \langle \mathbf{R}^{v,l} - \widetilde{G}^l, \delta_t^{(1)} \mathbf{e}^{v,l} \rangle\right| \leq 2\tau \sum_{l=0}^k \|\mathbf{R}^{v,l}\|_2^2 + C_2^v \|\mathbf{e}^{v,0}\|_2^2 + C_3^v \tau \sum_{l=0}^k \|\delta_t \mathbf{e}^{v,l}\|_2^2, \quad \forall k \in I_{N-1}. \tag{3.49}$$

Proof. We will only establish (3.46) and (3.48), the other inequalities are proved in similar way. Let C_0^u be the a bound of the second partial derivative of F with respect to u on $\mathbb{R}^2$. As a consequence of the

Mean Value Theorem and a straightforward integration, $|\widetilde{F}_j^k| \leq C_0(|\mathbf{e}_j^{u,k+1}| + |\mathbf{e}_j^{u,k-1}|)$ for each $j \leq \overline{J}$ and $k \in I_{K-1}$. It follows that

$$\begin{aligned} |2\langle \mathbf{R}^{u,k} - \widetilde{F}^k, \delta_t^{(1)}\varepsilon^n\rangle| &\leq 2\|\mathbf{R}^{u,k}\|_2^2 + 2\|\widetilde{F}^k\|_2^2 + \|\delta_t^{(1)}\mathbf{e}^{u,k}\|_2^2 \\ &\leq 2\|\mathbf{R}^{u,k}\|_2^2 + 4C_0^u\left(\|\mathbf{e}^{u,k+1}\|_2^2 + \|\mathbf{e}^{u,k-1}\|_2^2\right) + \frac{1}{2}\left(\|\delta_t\mathbf{e}^k\|_2^2 + \|\delta_t\mathbf{e}^{k-1}\|_2^2\right), \end{aligned} \tag{3.50}$$

whence the inequality (3.46) readily follows with $C_1^u = \max\{4C_0^u, \frac{1}{2}\}$. Using (3.50), we obtain now

$$\begin{aligned} 2\tau\left|\sum_{l=1}^{k}\langle \mathbf{R}^{u,l} - \widetilde{F}^l, \delta_t^{(1)}\mathbf{e}^{u,l}\rangle\right| &\leq 2\tau\sum_{l=0}^{k}\|\mathbf{R}^{u,l}\|_2^2 + 2C_1^u\tau\left[\sum_{l=0}^{k+1}\|\mathbf{e}^{u,l}\|_2^2 + \sum_{l=0}^{k}\|\delta_t\mathbf{e}^{u,l}\|_2^2\right] \\ &\leq 2\tau\sum_{l=0}^{k}\|\mathbf{R}^{u,l}\|_2^2 + 2C_1^u\tau\left[\sum_{l=0}^{k+1}\left(2\|\mathbf{e}^{u,0}\|_2^2 + 2T\tau\sum_{i=0}^{l-1}\|\delta_t\mathbf{e}^{u,i}\|_2^2\right) + \sum_{l=0}^{k}\|\delta_t\mathbf{e}^{u,l}\|_2^2\right] \\ &\leq 2\tau\sum_{l=0}^{k}\|\mathbf{R}^{u,l}\|_2^2 + 4C_1^uT\|\mathbf{e}^{u,0}\|_2^2 + 2C_1^u(2T^2+1)\tau\sum_{l=0}^{k}\|\delta_t\mathbf{e}^{u,l}\|_2^2, \quad \forall k \in I_{K-1}. \end{aligned} \tag{3.51}$$

The conclusion follows letting $C_2^u = 4C_1^uT$ and $C_3^u = 2C_1^u(2T^2+1)$. □

Next, we will use the notation $\Phi = (\phi^u, \phi^v, \psi^u, \psi^v)$ and $\tilde{\Phi} = (\phi^{\tilde{u}}, \phi^{\tilde{v}}, \psi^{\tilde{u}}, \psi^{\tilde{v}})$ to represent two sets of initial conditions for (3.6). In the following, the constants C_1^w, C_2^w and C_3^w will be as in Lemma 3.4.3, for each $w = u, v$.

Theorem 3.4.4 (Stability)**.** *Assume that $F, G \in \mathcal{C}^2(\mathbb{R}^2)$ have partial derivatives of the second order with respect to u and v, respectively, which are bounded in $\mathbb{R}^2$. Let*

$$\frac{1}{2}d_u\tau^2\gamma_h^{(\alpha_1)} + C_3^u\tau < \tau_u, \qquad \frac{1}{2}d_v\tau^2\gamma_h^{(\alpha_2)} + C_3^v\tau < \tau_v. \tag{3.52}$$

Suppose that $(\mathbf{u}, \mathbf{v})$ and $(\tilde{\mathbf{u}}, \tilde{\mathbf{v}})$ are solutions of (3.32) corresponding to Φ and $\tilde{\Phi}$, respectively, and define $\mathbf{e}^{u,k} = \mathbf{u}^k - \tilde{\mathbf{u}}^k$ and $\mathbf{e}^{v,k} = \mathbf{v}^k - \tilde{\mathbf{v}}^k$, for each $k \in \overline{I}_K$. Then there exist constants $C_4, C_5 \in \mathbb{R}^+$ such that

$$\begin{aligned} &\sum_{w=u,v}\|\delta_t\mathbf{e}^{w,k}\|_2^2 + \sum_{i\in I_2}\mu_t\left[\|\Lambda_{x_i}^{(\alpha_1)}\mathbf{e}^{u,k}\|_2^2 + \|\Lambda_{x_i}^{(\alpha_2)}\mathbf{e}^{v,k}\|_2^2\right] \leq \\ &\quad C_5\left(\sum_{w=u,v}\left[\|\delta_t\mathbf{e}^{w,0}\|_2^2 + \|\mathbf{e}^{w,0}\|_2^2\right] + \sum_{i\in I_2}\mu_t\left[\|\Lambda_{x_i}^{(\alpha_1)}\mathbf{e}^{u,0}\|_2^2 + \|\Lambda_{x_i}^{(\alpha_2)}\mathbf{e}^{v,0}\|_2^2\right]\right)e^{C_4k\tau}, \quad \forall k \in \overline{I}_K. \end{aligned} \tag{3.53}$$

Proof. It is obvious that the sequence $((\mathbf{e}^{u,k}, \mathbf{e}^{v,k}))_{k=0}^K$ satisfies

$$\begin{aligned} \tau_u\delta_t^{(2)}\mathbf{e}_j^{u,k} + \delta_t^{(1)}\mathbf{e}_j^{u,k} - \widetilde{F}_j^k - d_u\delta_x^{(\alpha_1)}\mathbf{e}_j^{u,k} &= 0, \quad \forall (j,k) \in \overline{J}\times I_{K-1}, \\ \tau_v\delta_t^{(2)}\mathbf{e}_j^{v,k} + \delta_t^{(1)}\mathbf{e}_j^{v,k} - \widetilde{G}_j^k - d_v\delta_x^{(\alpha_2)}\mathbf{e}_j^{v,k} &= 0, \quad \forall (j,k) \in \overline{J}\times I_{K-1}. \end{aligned}$$
$$\text{such that } \begin{cases} \mathbf{e}_j^{u,0} = \phi^u(x_j) - \phi^{\tilde{u}}(x_j), & \forall j \in \overline{J}, \\ \mathbf{e}_j^{v,0} = \phi^v(x_j) - \phi^{\tilde{v}}(x_j), & \forall j \in \overline{J}, \\ \mathbf{e}_j^{u,1} = \psi^u(x_j) - \psi^{\tilde{u}}(x_j), & \forall j \in \overline{J}, \\ \mathbf{e}_j^{v,1} = \psi^v(x_j) - \psi^{\tilde{v}}(x_j), & \forall j \in \overline{J}. \end{cases} \tag{3.54}$$

Here, we let $\widetilde{F}_j^k = \delta_{u,t}^{(1)}F_j^k(\mathbf{u}_j^k, \mathbf{v}_j^k) - \delta_{u,t}^{(1)}F_j^k(\tilde{\mathbf{u}}_j^k, \tilde{\mathbf{v}}_j^k)$ and $\widetilde{G}_j^k = \delta_{v,t}^{(1)}G_j^k(\mathbf{u}_j^k, \mathbf{v}_j^k) - \delta_{v,t}^{(1)}G_j^k(\tilde{\mathbf{u}}_j^k, \tilde{\mathbf{v}}_j^k)$, for each $(j,k) \in \overline{J}\times I_{K-1}$. On the other hand, note that the following identity is readily established:

$$\langle\delta_t^{(2)}\mathbf{e}^{w,k}, \delta_t^{(1)}\mathbf{e}^{w,k}\rangle = \frac{1}{2\tau}\left(\|\delta_t\mathbf{e}^{w,k}\|_2^2 - \|\delta_t\mathbf{e}^{w,k-1}\|_2^2\right), \quad \forall k \in I_{K-1}, \forall w = u, v. \tag{3.55}$$

Also, using the properties of square-root operators, we obtain that

$$\begin{aligned} \langle -\delta_x^{(\zeta)}\mathbf{e}^{w,k}, \delta_t^{(1)}\mathbf{e}^{w,k}\rangle = \frac{1}{2\tau}\sum_{i=1}^{2}[&\left(\mu_t\|\Lambda_{x_i}^{(\zeta)}\mathbf{e}^{w,k}\|_2^2 - \frac{\tau^2}{2}\|\Lambda_{x_i}^{(\zeta)}\delta_t\mathbf{e}^{w,k}\|_2^2\right) \\ &- \left(\mu_t\|\Lambda_{x_i}^{(\zeta)}\mathbf{e}^{w,k-1}\|_2^2 - \frac{\tau^2}{2}\|\Lambda_{x_i}^{(\zeta)}\delta_t\mathbf{e}^{w,k-1}\|_2^2\right)], \end{aligned} \tag{3.56}$$

for each $k \in I_K$, $w = u, v$ and $\zeta \in (0,1) \cup (1,2]$. Let $\eta_0^u \in \mathbb{R}^+$ satisfy $\frac{1}{2} d_u \tau^2 \gamma_h^{(\alpha_1)} < \eta_0^u < \tau_u - C_3^u \tau$, and define the constants

$$\omega^{u,k} = (\tau_u - C_3^u - \eta_0^u)\|\delta_t \mathbf{e}^{u,k}\|_2^2 + d_u \sum_{i \in I_2} \mu_t \|\Lambda_{x_i}^{(\alpha_1)} \mathbf{e}^{u,k}\|_2^2, \quad \forall k \in \overline{I}_{K-1}, \tag{3.57}$$

$$\rho^u = \tau_u \|\delta_t \mathbf{e}^{u,0}\|_2^2 + d_u \sum_{i \in I_2} \mu_t \|\Lambda_{x_i}^{(\alpha_1)} \mathbf{e}^{u,0}\|_2^2 + C_2^u \|\mathbf{e}^{u,0}\|_2^2. \tag{3.58}$$

Let $l \in I_K$, take the inner product of $\delta_t^{(1)} \mathbf{e}^{u,k}$ with both sides of the first difference equation of (3.54), and substitute the identities above. Multiply then by 2τ, sum then over all $k \in I_l$, use the inequality (3.48) with $\mathbf{R}^{u,k} = 0$ and the properties in Lemma 3.3.7, and simplify algebraically to obtain

$$\begin{aligned} \omega^l &\leq (\tau_u - C_3^u \tau)\|\delta_t \mathbf{e}^{u,l}\|_2^2 + d_u \sum_{i \in I_2} \mu_t \|\Lambda_{x_i}^{(\alpha_1)} \mathbf{e}^{u,l}\|_2^2 - \frac{1}{2} d_u \tau^2 \sum_{i \in I_2} \|\Lambda_{x_i}^{(\alpha_1)} \delta_t \mathbf{e}^{u,l}\|_2^2 \\ &\leq (\tau_u - C_3^u \tau)\|\delta_t \mathbf{e}^{u,0}\|_2^2 + d_u \sum_{i \in I_2} \mu_t \|\Lambda_{x_i}^{(\alpha_1)} \mathbf{e}^{u,0}\|_2^2 + 2\tau \left| \sum_{k=1}^{l} \langle \widetilde{F}^k, \delta_t^{(1)} \mathbf{e}^{u,k} \rangle \right| \\ &\leq \rho^u + C_3^u \tau \sum_{k=0}^{l-1} \|\delta_t \mathbf{e}^{u,k}\|_2^2 \leq \rho^u + C_4^u \tau \sum_{k=0}^{l-1} \omega^{u,k}, \quad \forall l \in I_{K-1}. \end{aligned} \tag{3.59}$$

Here, we used $C_4^u = C_3^u / (\tau_u - C_3^u \tau - \eta_0^u) \in \mathbb{R}^+$. An application of Lemma 3.4.2 shows that $\omega^{u,k} \leq \rho^u e^{C_4^u k\tau}$ for each $k \in \overline{I}_K$. Let $\eta_0^v \in \mathbb{R}^+$ satisfy $\frac{1}{2} d_v \tau^2 \gamma_h^{(\alpha_2)} < \eta_0^v < \tau_v - C_3^v \tau$, and define the constants

$$\omega^{v,k} = (\tau_v - C_3^v \tau - \eta_0^v)\|\delta_t \mathbf{e}^{v,k}\|_2^2 + d_v \sum_{i \in I_2} \mu_t \|\Lambda_{x_i}^{(\alpha_2)} \mathbf{e}^{v,k}\|_2^2, \quad \forall k \in \overline{I}_{K-1}, \tag{3.60}$$

$$\rho^v = \tau_v \|\delta_t \mathbf{e}^{v,0}\|_2^2 + d_v \sum_{i \in I_2} \mu_t \|\Lambda_{x_i}^{(\alpha_2)} \mathbf{e}^{v,0}\|_2^2 + C_2^v \|\mathbf{e}^{v,0}\|_2^2. \tag{3.61}$$

In similar fashion, it is easy to check that there exists $C_4^v \in \mathbb{R}^+$ such that $\omega^{v,k} \leq \rho^v e^{C_4^v k\tau}$ for each $k \in \overline{I}_K$. Let $C_4 = C_4^u \vee C_4^v$ and $\zeta = \min\{\tau_u - C_3^u \tau - \eta_0^u, \tau_v - C_3^v \tau - \eta_0^v, d_u, d_v\}$. It follows that

$$\zeta \left(\|\delta_t \mathbf{e}^{u,k}\|_2^2 + \|\delta_t \mathbf{e}^{v,k}\|_2^2 + \sum_{i \in I_2} \mu_t \left[\|\Lambda_{x_i}^{(\alpha_1)} \mathbf{e}^{u,k}\|_2^2 + \|\Lambda_{x_i}^{(\alpha_2)} \mathbf{e}^{v,k}\|_2^2 \right] \right) \leq \omega^{u,k} + \omega^{v,k} \leq (\rho^u + \rho^v) e^{C_4 k\tau} \tag{3.62}$$

The conclusion of the theorem follows now letting $C_5 = \zeta^{-1} \max\{\tau_u, \tau_v, d_u, d_v, C_2^u, C_2^v\}$. □

Theorem 3.3.9 established the existence of solutions of the method (3.32). We will prove the uniqueness next.

Corollary 3.4.5 (Uniqueness of solutions)**.** *Suppose that $F, G \in \mathcal{C}^2(\mathbb{R}^2)$ have bounded derivatives up to second order in $\mathbb{R}^2$, and let* (3.52) *be satisfied. Then* (3.32) *has a unique solution for any set of initial data.*

Proof. Suppose that $(\mathbf{u}, \mathbf{v})$ and $(\tilde{\mathbf{u}}, \tilde{\mathbf{v}})$ are solutions of (3.32) corresponding to the same set of initial data Φ. By hypothesis, $(\mathbf{u}^0, \mathbf{v}^0) = (\tilde{\mathbf{u}}^0, \tilde{\mathbf{v}}^0)$ and $(\mathbf{u}^1, \mathbf{v}^1) = (\tilde{\mathbf{u}}^1, \tilde{\mathbf{v}}^1)$, so let us assume that $(\mathbf{u}^k, \mathbf{v}^k) = (\tilde{\mathbf{u}}^k, \tilde{\mathbf{v}}^k)$ for some $k \in I_{K-1}$. The inequality (3.53) together with the fact that the identities

$$\|\delta_t \mathbf{e}^{w,0}\|_2 = \|\mathbf{e}^{w,0}\|_2 = \mu_t \|\Lambda_{x_i}^{(\alpha_1)} \mathbf{e}^{u,0}\|_2 = \|\Lambda_{x_i}^{(\alpha_2)} \mathbf{e}^{v,0}\|_2 = 0 \tag{3.63}$$

hold for each $w = u, v$ and $i \in I_2$, and the inequality

$$\|\delta_t \mathbf{e}^{u,k}\|_2^2 + \|\delta_t \mathbf{e}^{u,k}\|_2^2 \leq \sum_{w=u,v} \|\delta_t \mathbf{e}^{w,k}\|_2^2 + \sum_{i \in I_2} \mu_t \left[\|\Lambda_{x_i}^{(\alpha_1)} \mathbf{e}^{u,k}\|_2^2 + \|\Lambda_{x_i}^{(\alpha_2)} \mathbf{e}^{v,k}\|_2^2 \right], \tag{3.64}$$

yield that $\|\delta_t \mathbf{e}^{u,k}\|_2 = \|\delta_t \mathbf{e}^{u,k}\|_2 = 0$. As a consequence of the assumption on the solutions at the kth temporal step, we obtain that $(\mathbf{u}^{k+1}, \mathbf{v}^{k+1}) = (\tilde{\mathbf{u}}^{k+1}, \tilde{\mathbf{v}}^{k+1})$. The result follows now by induction. □

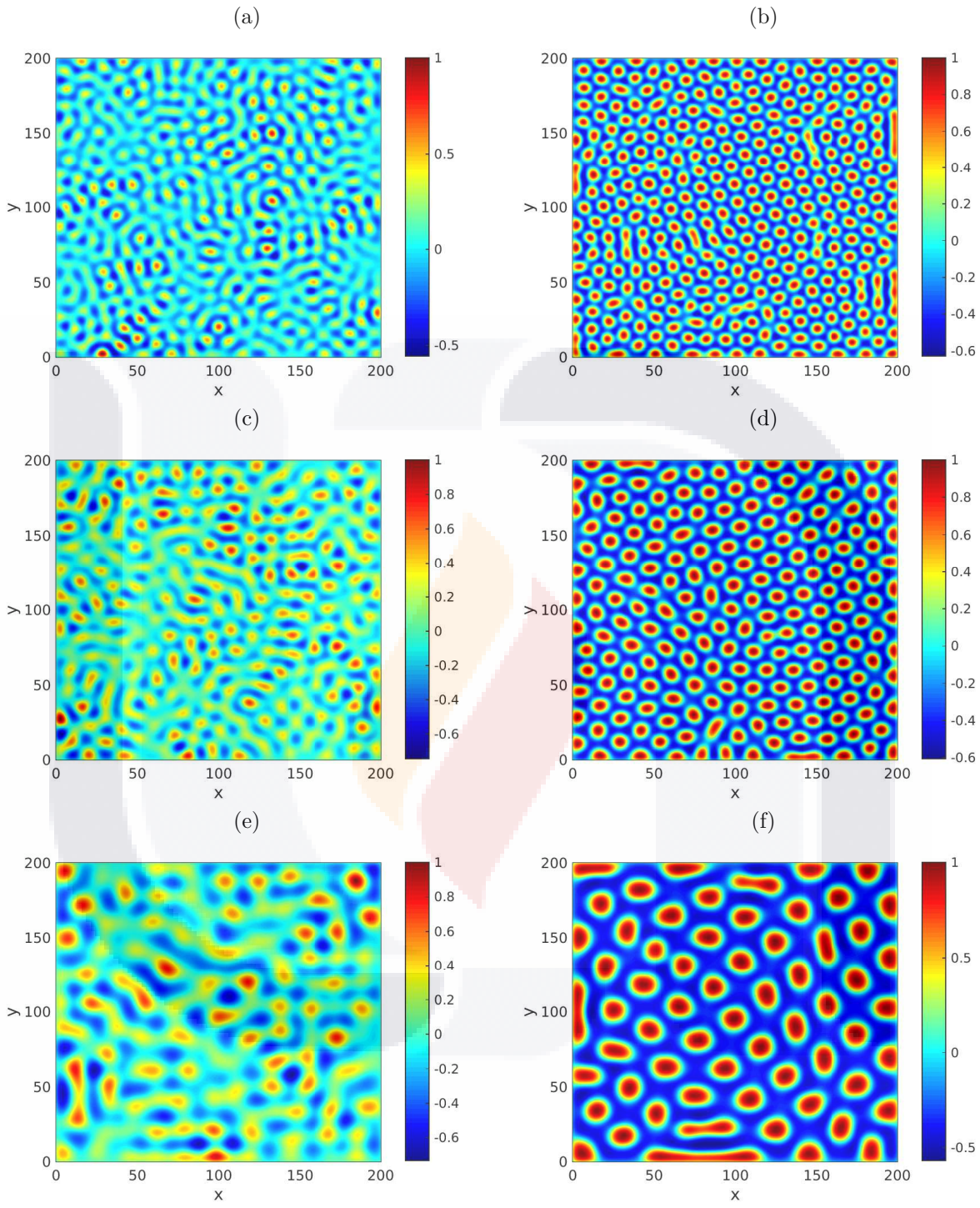

Figure 3.1: Snapshots of the approximate solutions of the variable u of (3.4) versus $(x, y) \in B = (0, 200) \times (0, 200)$ for $\alpha = \alpha_1 = \alpha_2$ and $\alpha = 2$ (top row), $\alpha = 1.5$ (middle row) and $\alpha = 1$ (bottom row). The times $t = 100$ (left column) and $t = 1000$ (right column) were used in these simulations, together with the parameter values $a = 7.45$, $b = 2.5$, $c = 5$, $d_u = 1$, $d_v = 20$ and $\tau_u = \tau_v = 1$. Computationally, we used the method (3.32) with the numerical constants $h_1 = h_2 = 1$ and $\tau = 0.01$. The graphs were normalized with respect to the absolute maximum of the solution at each time.

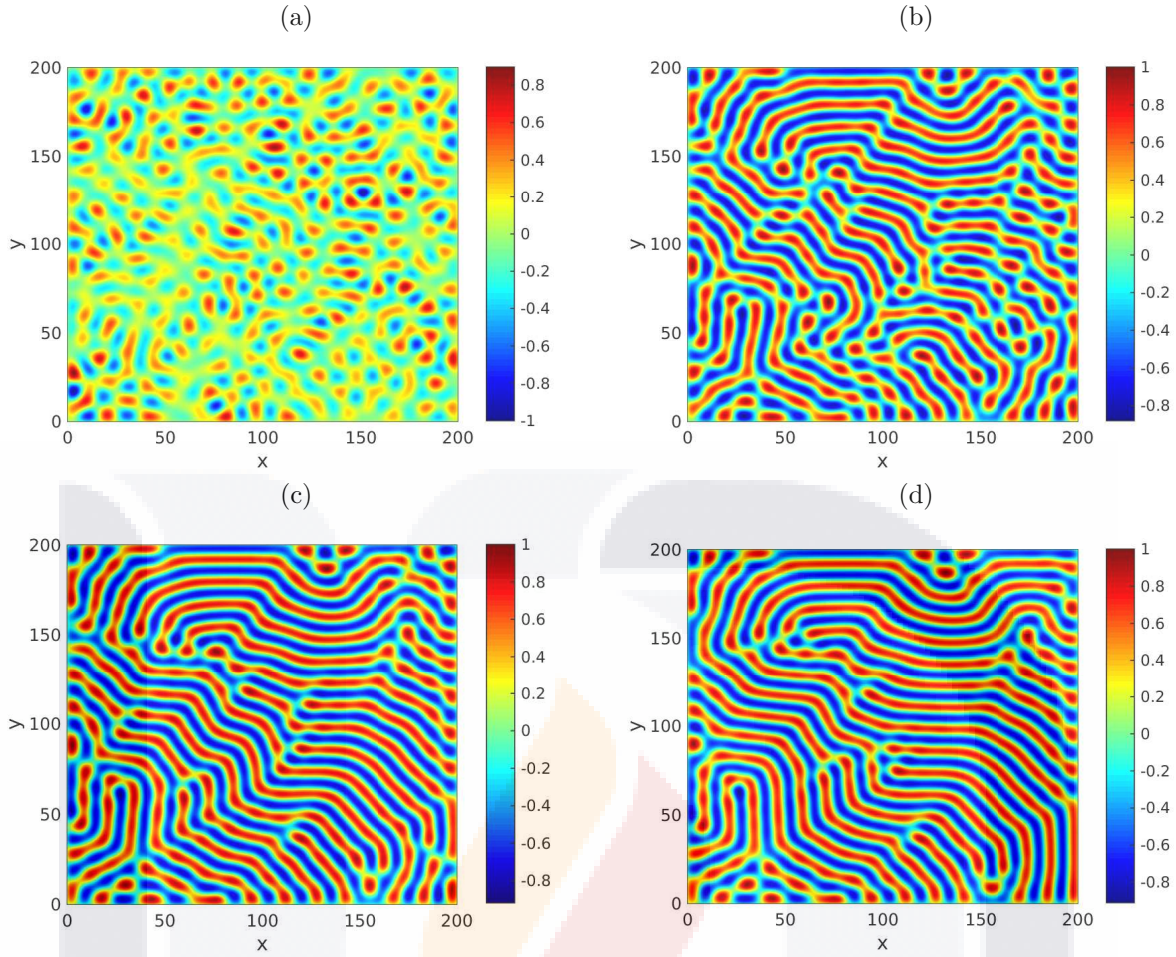

Figure 3.2: Snapshots of the approximate solutions of the variable u of (3.4) versus $(x, y) \in B = (0, 200) \times (0, 200)$ for $\alpha_1 = \alpha_2 = 1.5$. The times (a) $t = 100$, (b) $t = 400$, (c) $t = 1000$ and (d) $t = 2500$ were used in these simulations, together with the parameter values $a = 7.45$, $b = 0.5$, $c = 5$, $d_u = 1$, $d_v = 20$ and $\tau_u = \tau_v = 1$. Computationally, we used the method (3.32) with the numerical constants $h_1 = h_2 = 1$ and $\tau = 0.01$. The graphs were normalized with respect to the absolute maximum of the solution at each time.

Finally, the next result summarizes the convergence properties of (3.32). Its proof is similar to that of Theorem 3.4.4, for that reason we provide only a sketch of the proof.

Theorem 3.4.6 (Convergence)**.** *Suppose that $F, G \in \mathcal{C}^2(\mathbb{R}^2)$ have bounded derivatives up to second order in $\mathbb{R}^2$, and assume that* (3.52) *holds. If $u, v \in \mathcal{C}^5(\overline{\Omega})$ are solutions of* (3.6) *corresponding to the initial data Φ, then the method* (3.32) *converges to the exact solution with order $\mathcal{O}(\tau^2 + \|h\|_2^2)$.*

Proof. Let $(\mathbf{u}, \mathbf{v})$ be the unique solution of (3.32), and let $\mathbf{e}^{u,k} = u^k - \mathbf{u}^k$ and $\mathbf{e}^{v,k} = v^k - \mathbf{v}^k$, for each $k \in \overline{I}_K$. Note that the sequence $((\mathbf{e}^{u,k}, \mathbf{e}^{v,k}))_{k=0}^K$ satisfies

$$\begin{aligned} \tau_u \delta_t^{(2)} \mathbf{e}_j^{u,k} + \delta_t^{(1)} \mathbf{e}_j^{u,k} - \widetilde{F}_j^k - d_u \delta_x^{(\alpha_1)} \mathbf{e}_j^{u,k} &= \mathbf{R}_j^{u,k}, \quad \forall (j,k) \in \overline{J} \times I_{K-1}, \\ \tau_v \delta_t^{(2)} \mathbf{e}_j^{v,k} + \delta_t^{(1)} \mathbf{e}_j^{v,k} - \widetilde{G}_j^k - d_v \delta_x^{(\alpha_2)} \mathbf{e}_j^{v,k} &= \mathbf{R}_j^{u,k}, \quad \forall (j,k) \in \overline{J} \times I_{K-1}. \\ \text{such that: } \mathbf{e}_j^{u,0} = \mathbf{e}_j^{v,0} = \mathbf{e}_j^{u,1} = \mathbf{e}_j^{v,1} = 0, \quad \forall j \in \overline{J}. \end{aligned} \tag{3.65}$$

Here, we let $\widetilde{F}_j^k = \delta_{u,t}^{(1)} F_j^k(u_j^k, v_j^k) - \delta_{u,t}^{(1)} F_j^k(\mathbf{u}_j^k, \mathbf{v}_j^k)$ and $\widetilde{G}_j^k = \delta_{v,t}^{(1)} G_j^k(u_j^k, v_j^k) - \delta_{v,t}^{(1)} G_j^k(\mathbf{u}_j^k, \mathbf{v}_j^k)$, for each $(j,k) \in \overline{J} \times I_{K-1}$. The numbers $\mathbf{R}_j^{u,k}$ and $\mathbf{R}_j^{v,k}$ are the local truncation errors associated to the first and the second difference equations of (3.65), respectively. By Theorem 3.4.1, it follows that there exists $C \in \mathbb{R}^+$ such that $|\mathbf{R}_j^{u,k}|, |\mathbf{R}_j^{v,k}| \leq C(\tau^2 + \|h\|_2^2)$, for each $(j,k) \in \overline{J} \times \overline{I}_K$. It is easy to check that (3.55) and (3.56) are also satisfied in the present case. Let $\eta_0^u, \eta_0^v \in \mathbb{R}^+$ be as in the proof of Theorem 3.4.4, and

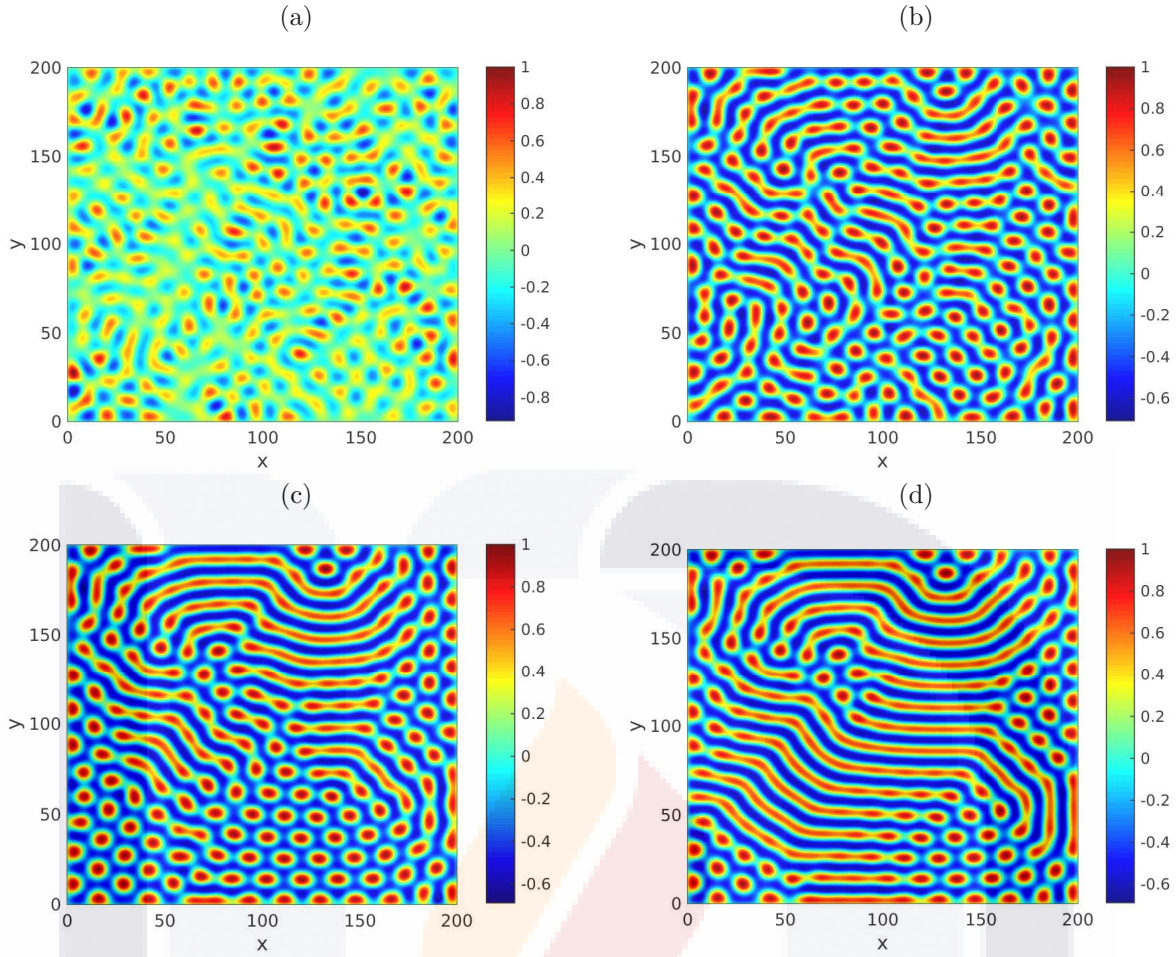

Figure 3.3: Snapshots of the approximate solutions of the variable u of (3.4) versus $(x, y) \in B = (0, 200) \times (0, 200)$ for $\alpha_1 = \alpha_2 = 1.5$. The times (a) $t = 150$, (b) $t = 450$, (c) $t = 1000$ and (d) $t = 2000$ were used in these simulations, together with the parameter values $a = 7.45$, $b = 1.5$, $c = 5$, $d_u = 1$, $d_v = 20$ and $\tau_u = \tau_v = 1$. Computationally, we used the method (3.32) with the numerical constants $h_1 = h_2 = 1$ and $\tau = 0.01$. The graphs were normalized with respect to the absolute maximum of the solution at each time.

let $C_4^w = C_3^w/(\tau_w - C_3^w\tau - \eta_0^w)$ for $w = u, v$. Let $\omega^{u,k}$ and $\omega^{v,k}$ be also as in the proof of Theorem 3.4.4, and define the constants

$$\rho^{u,k} = \tau_u\|\delta_t\mathbf{e}^{u,0}\|_2^2 + d_u\sum_{i\in I_2}\mu_t\|\Lambda_{x_i}^{(\alpha_1)}\mathbf{e}^{u,0}\|_2^2 + C_2^u\|\mathbf{e}^{u,0}\|_2^2 + \tau\sum_{l=0}^{k}\|\mathbf{R}^{u,l}\|_2^2, \quad \forall k \in \overline{I}_K, \tag{3.66}$$

$$\rho^{v,k} = \tau_v\|\delta_t\mathbf{e}^{v,0}\|_2^2 + d_v\sum_{i\in I_2}\mu_t\|\Lambda_{x_i}^{(\alpha_2)}\mathbf{e}^{v,0}\|_2^2 + C_2^v\|\mathbf{e}^{v,0}\|_2^2 + \tau\sum_{l=0}^{k}\|\mathbf{R}^{v,l}\|_2^2, \quad \forall k \in \overline{I}_K. \tag{3.67}$$

Note that we can use the initial conditions of (3.65) to simplify these last two expressions. Proceeding now as in the proof of Theorem 3.4.4, we obtain that $\omega^{u,k} \leq \rho^{u,k}e^{C_4^u k\tau}$ and $\omega^{v,k} \leq \rho^{v,k}e^{C_4^v k\tau}$ for each $k \in \overline{I}_K$. As a consequence, there exists $C_5 \in \mathbb{R}^+$ such that

$$\begin{aligned}\|\delta_t\mathbf{e}^{u,k}\|_2^2 + \|\delta_t\mathbf{e}^{v,k}\|_2^2 &\leq \|\delta_t\mathbf{e}^{u,k}\|_2^2 + \|\delta_t\mathbf{e}^{v,k}\|_2^2 + \sum_{i\in I_2}\mu_t\left[\|\Lambda_{x_i}^{(\alpha_1)}\mathbf{e}^{u,k}\|_2^2 + \|\Lambda_{x_i}^{(\alpha_2)}\mathbf{e}^{v,k}\|_2^2\right]\\ &\leq C_5(\rho^u + \rho^v)e^{C_4k\tau}\\ &\leq \tau C_5 e^{C_4T}\sum_{l=0}^{k}\left[\|\mathbf{R}^{u,l}\|_2^2 + \|\mathbf{R}^{v,l}\|_2^2\right] \leq C_6(\tau^2 + \|h\|_2^2)^2, \quad \forall k \in I_{K-1},\end{aligned} \tag{3.68}$$

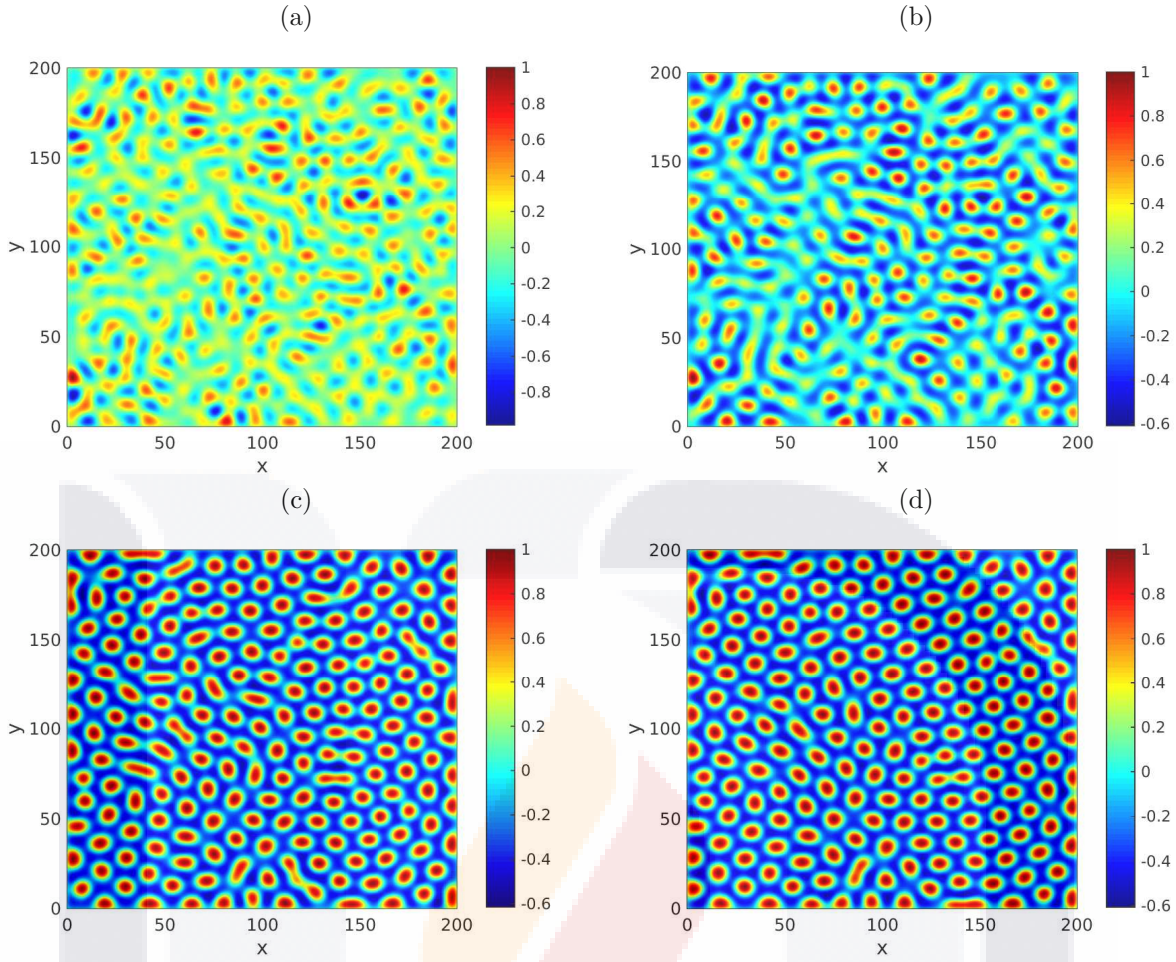

Figure 3.4: Snapshots of the approximate solutions of the variable u of (3.4) versus $(x, y) \in B = (0, 200) \times (0, 200)$ for $\alpha_1 = \alpha_2 = 1.5$. The times (a) $t = 50$, (b) $t = 150$, (c) $t = 450$ and (d) $t = 1000$ were used in these simulations, together with the parameter values $a = 7.45$, $b = 2.5$, $c = 5$, $d_u = 1$, $d_v = 20$ and $\tau_u = \tau_v = 3.5$. Computationally, we used the method (3.32) with the numerical constants $h_1 = h_2 = 1$ and $\tau = 0.01$. The graphs were normalized with respect to the absolute maximum of the solution at each time.

where $C_6 = 2C_5C^2Te^{C_4T}$. It is easy to see now that

$$\|\mathbf{e}^{w,k}\|_2^2 \leq 2\|\mathbf{e}^{w,0}\|_2^2 + 2T\tau \sum_{l=0}^{k-1} \|\delta_t \mathbf{e}^{w,l}\|_2^2 \leq C_7(\tau^2 + \|h\|_2^2)^2, \quad \forall k \in I_K, \forall w = u, v, \tag{3.69}$$

for $C_7 = 2T^2C_6$. We conclude that there exists $C_0 \in \mathbb{R}$ such that $\|\mathbf{e}^{w,k}\|_2 \leq C_0(\tau^2 + \|h\|_2^2)$ for each $k \in I_K$. The conclusion of the theorem readily follows from this fact. □

3.5 Numerical simulations

The first part of the present section is devoted to validate qualitatively the numerical method (3.32). To that end, we will consider the continuous model (3.4) defined on the set $B = (0, 200) \times (0, 200)$. Computationally, we let $h_1 = h_2 = 1$ and $\tau = 0.01$. The simulations were carried using an implementation of our method in ©Matlab 8.5.0.197613 (R2015a) on a ©Sony Vaio PCG-5L1P laptop computer with Linux Mint 18.03 Cinnamon (Sylvia) as operating system. In terms of computational times, we are aware that better results may be obtained with more modern equipment and more modest Linux/Unix distributions.

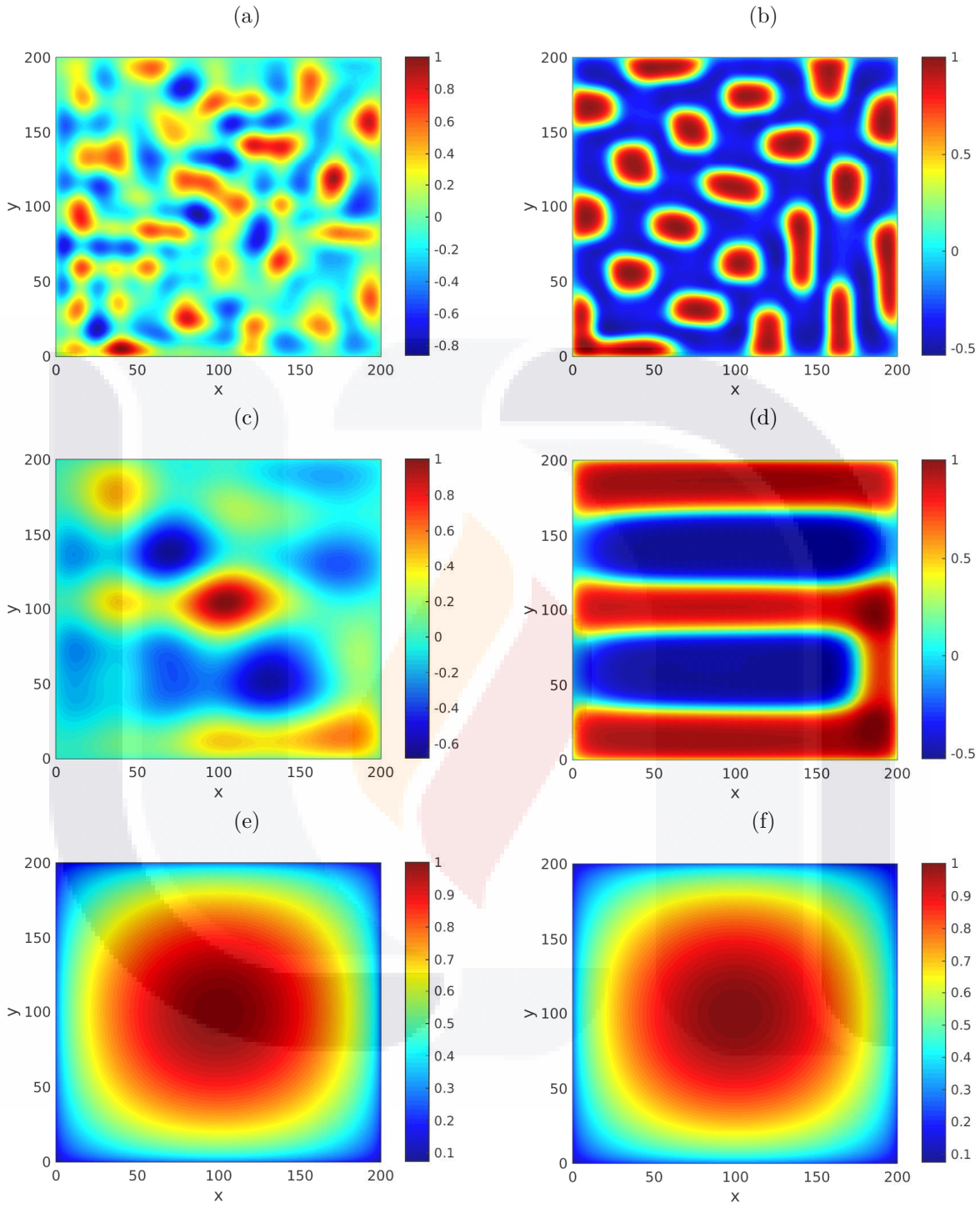

Figure 3.5: Snapshots of the approximate solutions of the variable u of (3.4) versus $(x, y) \in B = (0, 200) \times (0, 200)$ for $\alpha = \alpha_1 = \alpha_2$ and $\alpha = 0.75$ (top row), $\alpha = 0.50$ (middle row) and $\alpha = 0.25$ (bottom row). The times $t = 100$ (left column) and $t = 1000$ (right column) were used in these simulations, together with the parameter values $a = 7.45$, $b = 2.5$, $c = 5$, $d_u = 1$, $d_v = 20$ and $\tau_u = \tau_v = 3.5$. Computationally, we used the method (3.32) with the numerical constants $h_1 = h_2 = 1$ and $\tau = 0.01$. The graphs were normalized with respect to the absolute maximum of the solution at each time.

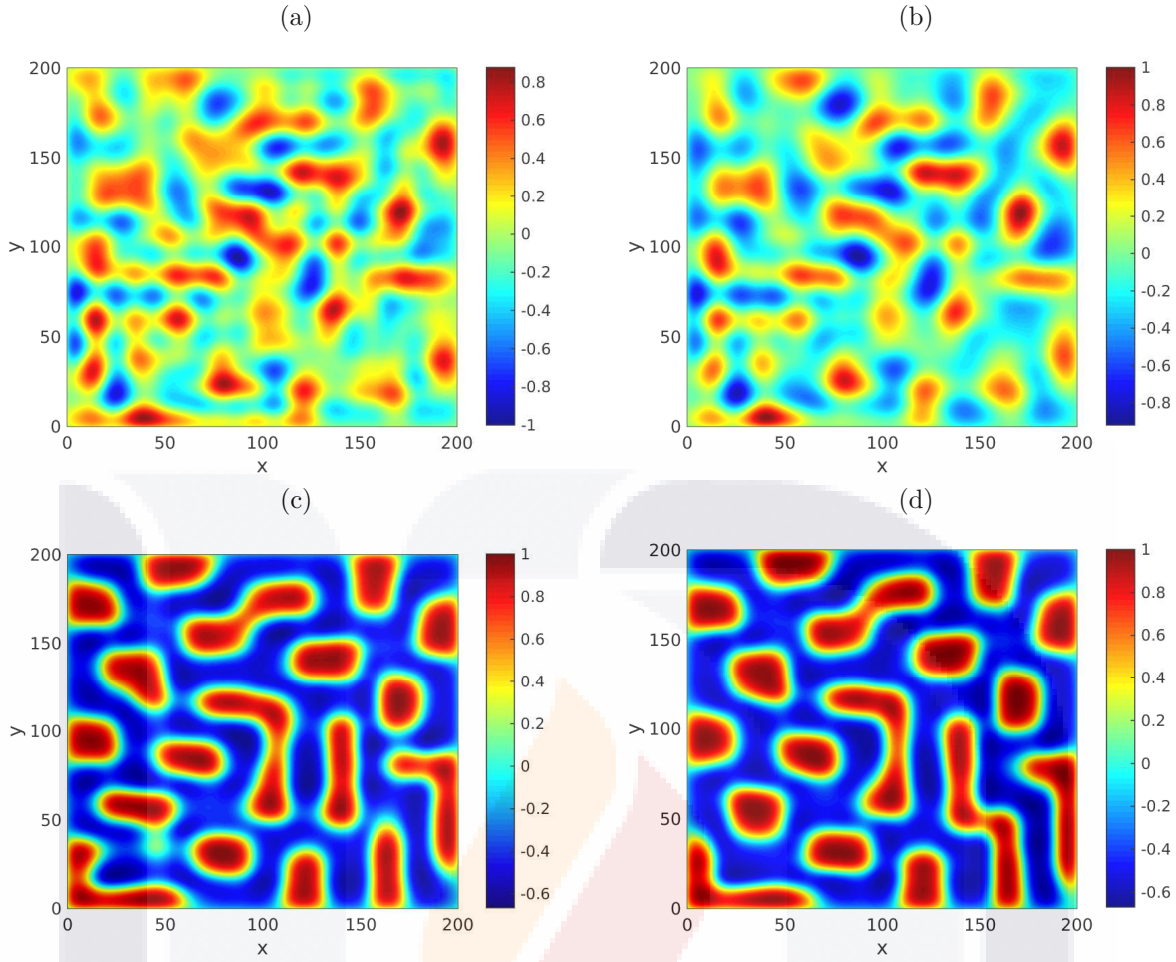

Figure 3.6: Snapshots of the approximate solutions of the variable u of (3.4) versus $(x, y) \in B = (0, 200) \times (0, 200)$ for $\alpha_1 = \alpha_2 = 0.75$. The times (a) $t = 50$, (b) $t = 100$, (c) $t = 400$ and (d) $t = 1000$ were used in these simulations, together with the parameter values $a = 7.45$, $b = 1.5$, $c = 5$, $d_u = 1$, $d_v = 20$ and $\tau_u = \tau_v = 1$. Computationally, we used the method (3.32) with the numerical constants $h_1 = h_2 = 1$ and $\tau = 0.01$. The graphs were normalized with respect to the absolute maximum of the solution at each time.

In the following, we let $\tau_u = \tau_v = \tau$, $d_u = 1$, $d_v = d$ and $\alpha = \alpha_1 = \alpha_2$. Moreover, we use parameter values satisfying (3.5), and let $x = x_1$ and $y = x_2$.

Example 3.5.1. Consider the system (3.4) with the parameter values $a = 7.45$, $b = 2.5$, $c = 5$, $d = 0.25$ and $\tau = 1$. As initial profiles, let ϕ^u and ϕ^v be samples of a uniformly distributed random variable on the interval $[-0.03, 0.03]$, and use zero initial velocities. Figure 3.1 shows snapshots of the approximate solutions of the variable u of (3.4) for various values of α and different times. We used $\alpha = 2$ (top row), $\alpha = 1.5$ (middle row) and $\alpha = 1$ (bottom row), together with the times $t = 100$ (left column) and $t = 1000$ (right column). These simulations establish that the wave number of Turing patters increases as the order of differentiation α increases, in agreement with the literature [89]. □

Example 3.5.2. Let $b = 0.5$, and consider all the other parameter values as in Example 3.5.1. Figure 3.2 shows snapshots of the approximate solutions of the variable u of (3.4) versus x and y for $\alpha = 1.5$. The times (a) $t = 150$, (b) $t = 450$, (c) $t = 1000$ and (d) $t = 2000$ were used in these simulations, and the graphs have been normalized with respect to the absolute maximum of the solution at each time. In this case, the solution firstly breaks up into hexagons due to the small perturbations at the initial time. The emergent hexagons are not stable, and they are replaced gradually by stripes. The stripes prevail over the whole domain, and the qualitative dynamics of the system does not undergo any further substantial changes. This is in agreement with the analytical results and with the parabolic scenario. □

Example 3.5.3. Fix now $b = 1.5$, and consider the same parameter values as in Example 3.5.2. Under these

circumstances, Figure 3.3 shows snapshots of the approximate solutions of the variable u of (3.4) versus x and y. We employed $\alpha = 1.5$, and the times (a) $t = 150$, (b) $t = 450$, (c) $t = 1000$ and (d) $t = 2000$. Notice that the results show the coexistence of strips and hexagons at different times. Ultimately, both the hexagonal and the striped patterns coexist. □

Example 3.5.4. Fix $b = 2.5$ and $\tau = 3$, while the remaining parameters are as in Example 3.5.2. Figure 3.4 shows snapshots of the approximate solutions of the variable u of (3.4) versus x and y for $\alpha = 1.5$, at the times (a) $t = 150$, (b) $t = 450$, (c) $t = 1000$ and (d) $t = 2000$. In our simulations, we noted the presence of stable hexagonal patterns at different times. Moreover, the pattern dynamics converges to stable hexagonal patterns. □

Our last example shows evidence supporting the existence of Turing patters in subdiffusive forms of (3.4).

Example 3.5.5. Use the same experimental setting of Example 3.5.1. Figure 3.5 shows snapshots of the approximate solutions of the variable u of (3.4) for various values of α and different times. We used $\alpha = 0.75$ (top row), $\alpha = 0.50$ (middle row) and $\alpha = 0.25$ (bottom row), together with the times $t = 100$ (left column) and $t = 1000$ (right column). These results show that Turing patters are also present in the system (3.4) when $\alpha \in (0, 1)$. Finally, Figure 3.6 shows the development of patterns in the system (3.4) when $\alpha = 0.75$. This behavior is similar to that obtained when $\alpha \in (1, 2]$. □

Conclusions

Chapter 2 In this chapter, we considered a damped fractional extension of the classical nonlinear wave equation. The model under investigation is defined on a closed and bounded interval of the real line, and it considers the presence of a general nonlinear potential function that generalizes many particular models from mathematical physics, including the well-known sine-Gordon and Klein–Gordon equations from relativistic quantum mechanics. Moreover, we considered a space-fractional extension of the wave equation using Riesz fractional derivatives of orders in $(1, 2)$. We show here that the model under investigation possesses energy functionals which are preserved under suitable assumptions on the boundary conditions and the parameters of the model. The exact resolution of the problem under study is a difficult mathematical task, so the design of numerical techniques that are capable of preserving discrete energy functions is a problem that merits further investigation.

Motivated by the analytical difficulties to provide explicit solutions of our fractional wave equation, we designed a finite-difference scheme to approximate its solutions. The numerical method is based on the use of fractional centered differences, which provide second-order consistent approximations of fractional-order derivatives. Using operator theory, we show that the discrete fractional Laplacian is a positive and self-adjoint operator, whence the existence of a square root readily follows. This fact is employed then to propose a discrete energy functional of the numerical method which, under suitable conditions on the boundary conditions and the model parameters, is preserved at each discrete time. Additionally, the method is a second-order consistent discretization of the problem under investigation, and the simulations provided in this work show that the energy is conserved throughout time when the assumptions of the relevant theorems on energy preservation are satisfied. Finally, we analyze the case of an unbounded domain, and we show that the same properties of conservation of energy hold in the unbounded case.

Chapter 3 In this chapter, we designed a numerical method to approximate the solutions of a two-dimensional hyperbolic system that describes the interaction between an activator and an inhibitor in chemical reactions. The system is nonlinear, and it consists of two coupled partial differential equations with polynomial reaction terms. We considered the presence of two-dimensional superdiffusive terms consisting of fractional operators of the Riesz type, with differentiation orders in $(0, 1) \cup (1, 2]$. Initial conditions were imposed on a closed and bounded rectangle of $\mathbb{R}^2$, and a finite-difference methodology based on the use of fractional centered differences was designed to approximate the solutions of the problem. We proved analytically the existence and the uniqueness of the solutions of the numerical method, and we established thoroughly the most interesting numerical properties of the method, namely, its quadratic consistency, its stability and its quadratic convergence. Some numerical simulations obtained through our method show the appearance of Turing patterns and wave instabilities, in agreement with some reports on superdiffusive models found in the literature. Moreover, the numerical simulations shows evidence supporting the existence of Turing patters also in subdiffusive forms of the physical model.

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