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На правах рукописи

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Конечно-разностные и спектрально-Галеркинские методы в моделях, описываемых дробными уравнениями в частных производных с запаздыванием

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Manuscript Rights

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FINITE-DIFFERENCE AND SPECTRAL-GALERKIN METHODS IN MODELS, DESCRIBED BY FRACTIONAL PARTIAL DIFFERENTIAL EQUATIONS WITH DELAY

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Mathematical Modeling, Numerical Methods and Software Packages

Dissertation is Submitted for the Degree of Candidate of Physical and Mathematical Sciences

> Scientific supervisor: Doc. of Phys. and Math. Sci., Professor Pimenov Vladimir Germanovich

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Introduction

The relevance of the topic and the degree of its development. Models described by fractional partial differential equations have developed into a potent instrument for mathematical modeling in recent years. The most important reasons why these models are favoured over integer-order models are their flexible representation and their ability to provide an accurate description of a wide range of phenomena. Delay time inclusion in fractional models allows for a more general representation and a more precise description of occurrences. The rationale behind this is because fractional derivatives, unlike ordinary ones, are non-local in nature and may be used to explain memory effects, whereas time delays disclose the history of a previous state. This kind of models are very useful for describing a variety of complicated systems and aberrant behavior in natural science and effectively applied in many fields including bioengineering, control theory, economics, electrochemistry, physics, quantum mechanics, etc. [1–20].

The Schnakenberg model, presented in 1979 [21], is a natural system of autocatalysis that often occurs in various biological systems and is considered one of the most significant biochemical reaction systems in modelling complex biological processes. This model describes an autocatalytic chemical reaction using the periodic oscillatory behavior of a morphogen's spatial distribution and also offers insights into how multiple morphogens react with cells and patterns. In these reactions, the reaction rate accelerates as the reaction proceeds. This type of situation arises when a product acts as a catalyst for the response, so the reaction rate goes up with time, and the chemical kinetic of the reaction becomes positive. Despite its importance, the Schnakenberg model has not received much attention from fractional representation. The majority of previous works which were presented used ordinary differential equations to describe this model, notably with the influence of time delay, including the works [22–25], of the following form:

$$\begin{cases} \frac{\partial \Phi_1}{\partial t} - \kappa_1 \frac{\partial \Phi_1^2}{\partial x^2} = f_1 \big(\Phi_1(x,t), \Phi_1(x,t-s), \Phi_2(x,t), \Phi_2(x,t-s) \big), & x \in \Omega, \ t \in I, \\ \frac{\partial \Phi_2}{\partial t} - \kappa_2 \frac{\partial \Phi_2^2}{\partial x^2} = f_2 \big(\Phi_1(x,t), \Phi_1(x,t-s), \Phi_2(x,t), \Phi_2(x,t-s) \big), & x \in \Omega, \ t \in I, \end{cases}$$

$$(1)$$

where $\Phi_1(x,t)$ and $\Phi_2(x,t)$ denote the species concentrations or densities at time t, κ_1, κ_2 represent the diffusion coefficients and s refer to the delay term.

Many real-world problems don't fit well with the classical models, which rely on integer order derivatives. For instance, these derivatives don't consider many physical properties of the variables and parameters involved in the system as well as the memory effects [26]. Fractional order models, in general, are a powerful tool for understanding the physical aspects of variables and parameters in models. To our knowledge, no study has yet been published investigating the numerical solutions of the nonlinear delayed Schnakenberg model described by fractional partial differential equations. This gap in the literature leads us to consider this case study.

The qualitative theory of fractional differential equations with an independent variable and fractional partial derivatives has been extensively investigated and developed in recent years; see, for instance, [27–32]. In addition, fractional-order partial differential equations are classified into two distinct categories, those having a fractional derivative in space and those with a fractional derivative in time. Several analytical approaches, such as the iteration method [33], the Fourier transform technique [34–36], the series method [37], the Laplace transform method [38–40], the Mellin transform method [41; 42], and other methods [43–47], have been utilized in the process of finding the exact and approximate analytic solutions to the fractional differential equations. Some of these techniques include a transformation to break down complex equations into smaller ones, while others provide the solution as a series that eventually converges into the exact solution. Notably, analytical methods are ineffective for the majority of fractional differential equations, particularly nonlinear problems.

However, due to the complexity of the problems and the inability of employing analytical approaches to find solutions, numerical methods come to the forefront. It's possible that Shanukov's works [48; 49] were the first ones in this area to be published. There followed a plethora of publications that built numerical methods for various classes of such equations, including finite difference methods [50–57], finite element methods [58–61] and other numerical methods [62–67]. On the other hand, spectral approaches have evolved rapidly in recent decades [68–71]. The primary benefit of spectral approaches is their ability to produce very precise results. The four most often used spectral methods are Galerkin, tau, collocation, and spectral element methods. The proper spectral approach proposed for solving such differential equations is obviously dependent on the kind of differential equation as well as the type of initial or boundary conditions governing it [72–74]. More detailed references related to such works, the results of which are used in the dissertation, are given in the introductions to each chapter.

Development of effective numerical algorithms for estimating the solutions of fractional delay partial differential equations (FDPDEs) has been a major problem in recent decades. A substantial cost in terms of numerical solvability is associated with the use of the memory effect of fractional derivatives in the development of basic material models or unified principles. In addition to other considerations, any method that uses a discretization of a non-integer derivative must take into account the non-local nature of the derivative, which generally results in a large storage need and high algorithmic complexity. Furthermore, the evolution of a dependent variable of FDPDEs impacts solving FDPDEs. The difficulty of solving FDPDEs comes from the dependence of that evolution at time t on their value at t - s where s is the time delay and all previous solutions due to the character of history dependence of a fractional derivative.

Notably, numerical techniques for time-fractional differential equations may be divided into two groups: indirect and direct approaches. Indirect methods work by reformulating time-fractional differential equations into integro-differential equations. In contrast, direct methods rely on direct estimates for time-fractional derivatives [75]. These methods include, for instance, the L1-difference formula [76] and the $L2 - 1_{\sigma}$ scheme [77]. The L1 schemes are constructed using piecewise polynomials that approximate time-fractional derivatives. Further information about the $L2-1_{\sigma}$ difference formula is detailed in the introduction of the chapter 3. Despite numerous numerical schemes employed for FDPDEs convergence and stability analysis for direct numerical methods of FDPDEs is limited especially for nonlinear problems [61; 78–81]. This is because of the unsuitable application of traditional techniques of discrete energy inequalities and the improper invoking of the traditional versions of discrete Grönwall inequalities. The nonlocality feature of time Caputo fractional derivatives and their singular kernels induced the interpolated numerical approximation for such kinds of derivatives. This makes the use of usual discrete Grönwall inequalities inappropriate. New versions of discrete Grönwall inequalities are recently constructed to fill this gap. These kinds of discrete inequalities are called discrete fractional Grönwall inequalities. They were firstly constructed by Liao and his coauthors in [82; 83] by introducing a new concept of discrete complementary convolution kernels corresponding to Riemann–Liouville fractional integral kernels.

It has been proved that these inequalities can be extended to FDPDEs [84–86]. This is done by deriving new forms, formulated in case of the appearance of discrete prehistory functions as a consequence of delay terms approximations.

Recent research has focused on developing alternative approaches to finding the approximate solution to FPDEs, as well as the appropriateness of the Legendre spectral method for other nonlinear models [87–90]. More recently, Zaky and Hendy introduced an intriguing technique for solving a class of one-dimensional nonlinear time-space fractional differential equations [91–94]. Specifically, the authors in [91] successfully combined the finite difference approximation of type L1 with the Legendre-Galerkin spectral method, to produce an efficient scheme for solving the non-linear time-space fractional diffusion equations of the following form:

$$\frac{\partial^{\beta}\Phi}{\partial t^{\beta}} = \kappa \frac{\partial^{\alpha}\Phi}{\partial |x|^{\alpha}} + f(x, t, \Phi(x, t)) + g(x, t), \quad x \in \Omega, \quad t \in I,$$
(2)

Additionally, by employing the same technique using the $L2 - 1_{\sigma}$ difference formula instead of the L1 formula, they were able to produce a high-order numerical scheme for the nonlinear time-space fractional Ginzburg-Landau equation in [93], and for coupled nonlinear time-space fractional Ginzburg-Landau complex system in [94]. These works are considered one of the first reports which combined the finite difference method with spectral schemes to develop numerical schemes for solving nonlinear fractional order problems.

Motivated by the aforementioned findings, developing and investigating novel numerical algorithms for solving models described by fractional partial differential equations is the first contribution of this dissertation. The other contribution is to extend that numerical and theoretical results to time-delay problems. According to the literature overview, as yet no study has used this technique to solve the nonlinear fractional models with delay. Despite the acknowledged considerable challenges such as nonlocality in time and space, as well as the nonlinearity of the problem under consideration, this lack of literature prompts us to investigate this case study.

Goals and tasks of the dissertation work. This dissertation is aimed at developing and substantiating numerical schemes for solving nonlinear fractional differential equations with fixed time delay. The main challenges of the considered work are represented in how to numerically approximate the time Caputo fractional derivative, Riesz space fractional derivatives, and the time delay to produce an easy-to-implement and consistent numerical scheme. The following are the main tasks of the dissertation work:

- (i) Develop and analyze a numerical method for solving the nonlinear time-space fractional-reaction diffusion equations with delay.
- (ii) Constructing and investigating a numerical method for solving the nonlinear multi-term time-space fractional-reaction diffusion equations with delay.
- (iii) Provide a novel numerical algorithm for solving fractional order Schnakenberg reaction-diffusion model with gene expression time delay.
- (iv) Design and develop a high-order numerical algorithm for solving the nonlinear time-space fractional-reaction diffusion equations with delay.
- (v) Include the substantiation of the stability and convergence of the developed algorithms and study of factors influencing the convergence orders.
- (vi) Provide numerical experiments to illustrate the computational efficiency and the theoretical results for the proposed methods.

Scientific novelty of the dissertation findings lies in the development of novel numerical algorithms to deal with nonlinear mathematical models that involve time delay effect and fractional derivatives in both time and space. In further detail, we briefly highlight the following:

- (i) An explicit numerical method for solving the nonlinear time-space fractional re action-diffusion equations with a fixed delay is constructed. The method is based on combining the L1 difference formula and the Legendre-Galerkin spectral method in order to discretize the temporal and space-fractional derivatives, respectively. The primary benefit of the suggested method is that the iterative approach is implemented linearly. The developed scheme has a 2β order for time if the solution is smooth enough and deteriorates to β order in the case of a non-smooth solution.
- (ii) An efficient hybrid numerical scheme for solving the generalized nonlinear multi-term time-space fractional reaction-diffusion equation with delay is constructed and developed. The methodology relies on novel algorithm which combine the L1 difference formula and Legendre-Galerkin spectral approach to discretize the time and space-fractional derivatives, respectively. The approach that has been suggested is stable and has a convergent order of $2 \beta_m$ in time, while simultaneously having an exponential rate of convergence in space.

- (iii) For the first time in literature, the analysis and numerical solutions of a generalized form of fractional-order Schnakenberg reaction-diffusion model with gene expression time delay are presented and discussed. This model is a natural system of autocatalysis, which is considered one of the direct applications of the delayed fractional diffusion equations in modelling of complex biological processes. By developing an efficient numerical technique to approximating Riesz-space and Caputo-time fractional orders, we achieved the numerical solutions. The approach is unconditionally stable with a 2β time convergent order and an exponential space convergence rate.
- (iv) High-order approximation for solving the nonlinear time-space fractional reaction-diffusion equations with time delay is constructed. The suggested algorithm depends on a combination of the $L2 - 1_{\sigma}$ difference formula and Legendre-Galerkin spectral approach to discretize both the time and space-fractional derivatives, respectively. Also, it is shown that the numerical scheme is unconditionally stable, with a second-order time-convergence and a space-convergent order of exponential rate.

Theoretical and practical significance of the work. Fractional partial equations with the additional effect of time delay, in general, are a powerful tool and play an important role in describing various phenomena in science and technology. The theoretical significance of the work lies in the development and study of new numerical methods for solving classes of equations in fractional derivatives both in time and in space, with a time delay effect. In addition, obtaining unambiguous conditions to ensure the stability and convergence of these methods. On other hand, the practical significance of the work lies in the possible application of the work results to study complex models of anomalous transport using computer experiments. It is also possible to use the developed numerical algorithms to model other phenomena described by similar FPDEs, such as semiconductor research and complex biological processes.

Methodology and research methods. The research builds on ideas and techniques from the rapidly growing field of numerical methods for solving partial differential equations; for examples, consult the works [95–100]. To complete the dissertation's tasks research, mathematical methods and computer algorithms side-by-side to computational schemes were used. More precisely, numerical methods were built using finite difference formulas of type L1 or $L2 - 1_{\sigma}$ together with the Galerkin–Legendre spectral technique for solving nonlinear fractional partial differential equations with time delay. For the theoretical analysis, convergence and stability estimates for the proposed schemes introduced in this work are investigated using discrete energy methodology inspired by recent discrete fractional Grönwall inequalities [84–86]. For numerical simulations, the Wolfram Mathematica programming language (version: 12.1) was used to design a set of programs based on the proposed computational algorithms.

Defense provisions. The following are the main results that can be attributed to the work done on the dissertation, all of which are original:

- (i) Develop and substantiate numerical method for solving the nonlinear Riesz-space and Caputo-time fractional reaction-diffusion equation with a fixed delay. A combined numerical scheme was constructed using the wellknown L1 difference approximation with Legendre Galerkin spectral approximation. The key advantage of the proposed method is that the implementation of the iterative approach is linear. The stability and the convergence of the semi-discrete scheme are proved by invoking the discrete fractional Halanay inequality. The stability and convergence of the fully discrete scheme are also investigated utilizing discrete fractional Grönwall inequalities, which show that the proposed method is stable and convergent. The results of the computational experiments carried out are consistent with the theoretical ones.
- (ii) Develop and substantiate numerical method for solving the generalized nonlinear multi-term time-space fractional reaction-diffusion equations with delay. A novel numerical scheme combines the Galerkin–Legendre spectral schemes, and a uniform L1-type interpolation technique is designed. The theoretical analysis of the constructed fully discrete scheme is successfully estimated using appropriate discrete fractional Grönwall inequalities, and the scheme is proven to be unconditionally stable and convergent. The theoretical results are in agreement with the outcomes of the computer experiments.
- (iii) Develop and substantiate numerical method for solving the fractional order equation in time and space with a delay of the general form of Schnakenberg model. A novel numerical approach is developed to approximately solve for Riesz-space and Caputo-time fractional orders, yielding the numerical

solutions. The described method is shown to be unconditionally stable, with a $2 - \beta$ convergent order in time and an exponential rate of convergence in space. The error estimates for the obtained solution are derived by applying a proper discrete fractional Grönwall inequality. The numerical simulations are performed and shown that are consistent with the expected theoretical.

(iv) Develop and substantiate high-order numerical algorithm for solving the nonlinear time-space fractional reaction-diffusion equations with delay. A novel scheme is proposed that mixes the Alikhanov $L2 - 1_{\sigma}$ difference formula with Galerkin spectral Legendre approach. It has been shown theoretically that the suggested scheme's numerical solution is unconditionally stable, with a second-order time-convergence and a space-convergent order of exponential rate. The numerical experiments that were performed agree with the theoretical predictions.

Personal contribution of the author. All the major scientific results of this dissertation were achieved by the author personally and are represented in the joint works with the co-authors (Ahmed S Hendy, Mahmoud A Zaky, and Vladimir G. Pimenov) [101–104].

Degree of reliability and approbation of results. The reliability of the results obtained in the work is confirmed by appropriate mathematical proofs, as well as numerical experiments conducted on test examples. Moreover, the main results of the work were discussed at seminars of the Department of Computational Mathematics and Computer Science of the Institute of Natural Sciences and Mathematics of the Ural Federal University, named after the first President of Russia B.N. Yeltsin and also presented at the following conferences:

52nd and 53rd All-Russian Schools-conferences with international participation "Modern problems of mathematics and its applications" (Yekaterinburg, Institute of Mathematics and Mechanics named after Academician N.N. Krasovsky, Ural Branch of the Russian Academy of Sciences, 2021 and 2022. https://sopromat.imm.uran.ru/ListReports).

Author's publications on the dissertation topic. The results of this dissertation are formulated in 4 articles [101–104] in peer-reviewed journals indexed by the Scopus and Web of Science:

- Omran, AK and Zaky, MA and Hendy, AS and Pimenov, VG An Efficient Hybrid Numerical Scheme for Nonlinear Multiterm Caputo Time and Riesz Space Fractional-Order Diffusion Equations with Delay // Journal of Function Spaces. 2021. V. 2021. Article ID 5922853. P. 1–13. https://doi.org/10.1155/2021/5922853
- Omran, AK and Zaky, MA and Hendy, AS and Pimenov, VG An easy to implement linear numerical scheme for fractional reaction-diffusion equations with prehistorical nonlinear source function // Mathematics and Computers in Simulation. 2022. V. 200. P. 218–239. https://doi.org/10.1016/j.matcom.2022.04.014
- Omran, AK and Zaky, MA and Hendy, AS and Pimenov, VG Numerical algorithm for a generalized form of Schnakenberg reaction-diffusion model with gene expression time delay// Applied Numerical Mathematics. 2023. V. 185. P. 295–310.

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In addition, the following computer program was officially registered at the Russian Federal Service for Intellectual Property:

5. Ibrahim Abdelrahim Khalifa Omran , Hendy Ahmed Said Abdelaziz, Ibrahim Mahmoud Abdelsalam Zaky. An easy-to-implement linear numerical scheme for fractional reaction-diffusion equations with a prehistoric nonlinear source function // Certificate of state registration of a computer program No. 2022613332. Registered in the Register of computer Programs of the Federal Service for Intellectual Property of Russia on March 14, 2022.

Structure and volume of the dissertation. The dissertation work consists of an introduction, four chapters, a conclusion, a list of references, a list of figures, and a list of tables. The dissertation manuscript contains 135 pages of the main text, 13 figures, 8 tables, and 190 references titles.

Overview of the dissertation. The out lines of this dissertation is organized as follows. In the rest of the introduction, we briefly review some notations, definitions, and preliminary facts that will be used further in this study. The main part of the research is presented in chapters 1-5 of the dissertation, which structurally and functionally corresponds to the stages of the implementation of the full cycle of the computational experiment.

Chapter 1 is dedicated to development the numerical method for solving the nonlinear time-space fractional reaction-diffusion equations with delay. We briefly review some results of earlier works that is relevant to the problem under consideration, after which the research challenge is formulated in section 1.1. We show the steps to build a fully discrete scheme on a uniform mesh in section 1.2. The main theoretical results of the chapter are presented by Theorem 1.1 and Theorem 1.2 in section 1.3, and by Theorem 1.3 and Theorem 1.4 in section 1.4. Finally, numerical experiments are provided in Section 1.5 to illustrate the convergence analysis of the obtained scheme.

Chapter 2 is devoted to designing numerical method for solving the generalized nonlinear multi-term time-space fractional reaction-diffusion equations with delay. Section 2.1 provides a brief summary of prior works related to the consideration problem, followed by the formulation of the problem. The steps needed to construct a fully discrete scheme on a uniform mesh are detailed in Section 2.2. Theorem 2.1 and Theorem 2.2 present the principal theoretical findings of the chapter in Section 2.3. Finally, numerical experiments are performed in Section 2.4 to illustrate the convergence analysis of the proposed approach.

Chapter 3 is devoted to studying a novel numerical algorithm for solving a generalized form of Schnakenberg reaction-diffusion model with time delay. Following a brief description of relevant prior work, we present the research problem formulation in Section 3.1. On a uniform mesh, we explain in Section 3.2 how to construct the fully discrete L1-Galerkin spectral scheme for the Schnakenberg model. The main theoretical findings of this chapter are shown in Section 3.3 by Theorem 3.1 and Theorem 3.2. Finally, numerical tests that support the convergence analysis of the proposed system are presented in Section 3.4.

Chapter 4 presents an effective high-order numerical method for solving the nonlinear time-space fractional reaction-diffusion equations with time delay. We first in Section 4.1 evaluate a summary of earlier research that is relevant to the discussion

of the study, after which the problem formulation is given. On a uniform mesh, we detail in Section 4.2 the way to construct the fully discrete Galerkin spectral scheme for the problem under consideration. Theorem 4.1 and Theorem 4.2 offer the most important theoretical results of this chapter in Section 4.3. Finally, Section 4.4 includes a numerical test that validates the obtained scheme's convergence analysis.

Chapter 5 is devoted to the description of software packages that allow conducting computer experiments for the numerical study of models described by fractional partial differential equations. Four software packages have been developed corresponding to the algorithm under study. Furthermore, examples are presented to further show how the dynamics of the solution to delayed models described by fractional partial differential equations are affected by fractional orders in the temporal and spatial directions.

Preliminaries

Here, we briefly recall some fundamental concepts and definitions in fractional calculus. For further details and complete introductions, we refer to the references [76; 105–110]. Following that, we go through the fundamental characteristics of Jacobi polynomials. We only introduce the facts which are needed for the purpose of numerical and theoretical investigations in this dissertation.

0.1 Basic concepts and notations.

We first fix the following notations for the sake of clearness during the sequel of this study. Let $\Omega = [a, b] \subset \mathbb{R}$ and $I = [0,T] \subset \mathbb{R}$ be the space and time domains respectively. In the following, we will assume that $\Phi : \Omega \times I \to \mathbb{R}$ is a sufficiently smooth function defined on the spatial domain Ω . Assume that $(\cdot, \cdot)_{0,\Omega}$ refer the standard inner product related to $L^2(\Omega)$ space with the usual L^2 norm and the maximum norm $\|\cdot\|_{\infty}$. Define the space $C_0^{\infty}(\Omega)$ consists of all smooth functions that have compact support in Ω . Consider that $H^r(\Omega)$ and $H_0^r(\Omega)$ are the standard Sobolev spaces, and their associated norms and seminorms, respectively, are $\|\cdot\|_r$ and $|\cdot|_r$. To further clarify, we characterize the approximation space \mathcal{W}_N^0 as

$$\mathcal{W}_N^0 = \mathcal{P}_N(\Omega) \cap H_0^1(\Omega),$$

where $\mathcal{P}_N(\Omega)$ denote the set of all polynomials of degree no more than N defined on the domain Ω . The interpolation operator of type Legendre-Gauss-Lobatto depicted by the symbol $I_N : C(\bar{\Omega}) \to \mathcal{W}_N$, can be defined as follows

$$\Phi(x_k) = I_N \Phi(x_k) \in \mathcal{P}_N, \quad k = 0, 1, \dots, N.$$

Definition 0.1 (Integro-differential operator). Let a and b be the boundaries of operations of order $\alpha \in \mathbb{R}$, then the continuous integro-differential operator can be defined as [109]

$${}_{a}D_{b}^{\alpha} = \begin{cases} \frac{d^{\alpha}}{dt^{\alpha}}, & \alpha > 0; \\ 1, & \alpha = 0; \\ \int_{a}^{b} (d\tau)^{\alpha}, & \alpha < 0. \end{cases}$$
(3)

Definition 0.2. The spatial left and the right Riemann–Liouville fractional partial derivatives of order $n - 1 < \alpha < n \in \mathbb{N}$ are defined, respectively, as [105]

$${}_{-\infty}D_x^{\alpha}\Phi(x,t) = \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_{-\infty}^x (x-\tau)^{n-1-\alpha}\Phi(\tau,t)d\tau,$$
(4)

$${}_{x}D^{\alpha}_{\infty}\Phi(x,t) = \frac{(-1)^{n}}{\Gamma(n-\alpha)}\frac{\partial^{n}}{\partial x^{n}}\int_{x}^{\infty}(\tau-x)^{n-1-\alpha}\Phi(\tau,t)d\tau,$$
(5)

where $\Gamma(x)$ symbolizes the usual gamma function. This allows us to give a definition for the Riesz space of fractional derivatives, which is [110]

$$\frac{\partial^{\alpha}\Phi}{\partial|x|^{\alpha}} = -c_{\alpha} \left({}_{a}D_{x}^{\alpha}\Phi(x,t) + {}_{x}D_{b}^{\alpha}\Phi(x,t) \right), \quad c_{\alpha} = \frac{1}{2\cos\frac{\pi\alpha}{2}}, \quad 1 < \alpha < 2.$$

Definition 0.3. The Caputo derivative of order β is defined as

$${}_{0}^{C}D_{t}^{\beta}\Phi(x,t) = \frac{\partial^{\beta}}{\partial t^{\beta}}\Phi(x,t) = \frac{1}{\Gamma(1-\beta)}\int_{0}^{t}(t-r)^{-\beta}\frac{\partial}{\partial r}\Phi(x,r)dr, \quad 0 < \beta < 1.$$
(6)

Definition 0.4 (Left fractional derivative space). For a given $\varepsilon > 0$, we define the following semi-norm and norm, respectively, as

$$\|\Phi\|_{J_{L}^{\varepsilon}(\Omega)} = \|_{a} D_{x}^{\varepsilon} \Phi\|_{0,\Omega}, \quad \|\Phi\|_{J_{L}^{\varepsilon}(\Omega)} = \left(\|\Phi\|_{J_{L}^{\varepsilon}}^{2}(\Omega) + \|\Phi\|_{0,\Omega}^{2}\right)^{1/2},$$

also, we define J_L^{ε} and $J_{L,0}^{\varepsilon}$ as the closures of $C^{\infty}(\Omega)$ and $C_0^{\infty}(\Omega)$, respectively, with respect to $\|\cdot\|_{J_L^{\varepsilon}(\Omega)}$.

Definition 0.5 (Right fractional derivative space). For a given $\varepsilon > 0$, we define the following semi-norm and norm, respectively, as

$$|\Phi|_{J_R^{\varepsilon}(\Omega)} = ||_x D_b^{\varepsilon} \Phi ||_{0,\Omega}, \quad ||\Phi||_{J_R^{\varepsilon}(\Omega)} = \left(|\Phi|_{J_R^{\varepsilon}(\Omega)}^2 + ||\Phi||_{0,\Omega}^2 \right)^{1/2},$$

also, we define J_R^{ε} and $J_{R,0}^{\varepsilon}$ as the closures of $C^{\infty}(\Omega)$ and $C_0^{\infty}(\Omega)$, respectively, with respect to $\|\cdot\|_{J_R^{\varepsilon}(\Omega)}$.

Definition 0.6 (Symmetric fractional derivative space). For a given $\varepsilon > 0$, such that $\varepsilon \neq n - \frac{1}{2}$, $n \in \mathbb{N}$, then we define the following semi-norm and norm, as

$$\mid \Phi \mid_{J_s^{\varepsilon}(\Omega)} = \mid (_a D_x^{\varepsilon} \Phi, _x D_b^{\varepsilon} \Phi)_{0,\Omega} \mid^{1/2}, \quad \left\| \Phi \right\|_{J_s^{\varepsilon}(\Omega)} = \left(\mid \Phi \mid_{J_s^{\varepsilon}}^2 (\Omega) + \left\| \Phi \right\|_{0,\Omega}^2 \right)^{1/2},$$

also, we define J_s^{ε} and $J_{s,0}^{\varepsilon}$ as the closures of $C^{\infty}(\Omega)$ and $C_0^{\infty}(\Omega)$, respectively, with respect to $\|\cdot\|_{J_s^{\varepsilon}(\Omega)}$.

Definition 0.7 (Fractional Sobolev space). For a given $\varepsilon > 0$, the fractional Sobolev space $H^{\varepsilon}(\Omega)$ is defined as

$$H^{\varepsilon}(\Omega) = \left\{ \Phi \in L^{2}(\Omega) \left| |\omega|^{\varepsilon} \mathcal{F}(\hat{\Phi}) \in L^{2}(\mathbb{R}) \right\},\right.$$

with respect to following semi-norm and norm, respectively, as

$$|\Phi|_{H^{\varepsilon}(\Omega)} = \left\| |\omega|^{\varepsilon} \mathcal{F}(\hat{\Phi}) \right\|_{0,\mathbb{R}}, \quad \|\Phi\|_{H^{\varepsilon}(\Omega)} = \left(|\Phi|^{2}_{H^{\varepsilon}(\Omega)} + \|\Phi\|^{2}_{0,\Omega} \right)^{1/2},$$

where $\mathcal{F}(\hat{\Phi})$ stands for the Fourier transformation for the function $\hat{\Phi}$, which represents the extension of zero of the function Φ outside of the spatial domain Ω . Also, we define $H^{\varepsilon}(\Omega)$ and $H_{0}^{\varepsilon}(\Omega)$ as the closures of $C^{\infty}(\Omega)$ and $C_{0}^{\infty}(\Omega)$, respectively, with consideration to $\|\cdot\|_{H^{\rho}(\Omega)}$.

Remark 0.1. According to the definitions above, if $\varepsilon \neq n - \frac{1}{2}$, $n \in \mathbb{N}$, then the fractional derivative spaces J_L^{ε} , J_R^{ε} , J_s^{ε} and H^{ε} are equivalent, with equivalent semi-norms and norms.

The adjoint property, which we will revisit below, will play a crucial part in the following study.

Lemma 0.1. For a given $\varepsilon > 0$, such that $1 < \varepsilon < 2$, then for any two functions $\Phi \in H_0^{\varepsilon}(\Omega)$ and $\upsilon \in H_0^{\varepsilon/2}(\Omega)$, the following relation is satisfied

$$({}_{a}D_{x}^{\varepsilon}\Phi,\upsilon)_{0,\Omega} = \left({}_{a}D_{x}^{\varepsilon/2}\Phi,{}_{x}D_{b}^{\varepsilon/2}\upsilon\right)_{0,\Omega}, \quad ({}_{x}D_{b}^{\varepsilon}\Phi,\upsilon)_{0,\Omega} = \left({}_{x}D_{b}^{\varepsilon/2}\Phi,{}_{a}D_{x}^{\varepsilon/2}\upsilon\right)_{0,\Omega}.$$
 (7)

0.2 Jacobi polynomials

Among the most important facets regarding fractional derivatives is the connection between their definitions and those of the Jacobi weights and the non-local kernel. In light of this fact, Jacobi polynomials play a vital role in the development of highly efficient spectral methods for fractional partial differential equations. So, we here introduce some fundamental properties of Jacobi polynomials. We recommend reading [99; 111] for more information on orthogonal polynomials, and [112–117] for applications of spectral methods to these type of polynomials. **Definition 0.8** (Jacobi polynomials). For p, q > -1 and $x \in (-1,1)$, the hypergeometric functions make it possible to define the Jacobian polynomials $J_0^{p,q}(x)$ as follows [99]:

$$J_0^{p,q}(x) = \frac{(p+1)i}{i!} {}_2F_1\left(-i, p+q+i+1; p+1; \frac{1-x}{2}\right), \quad i \in \mathbb{N},$$
(8)

where $(\cdot)_i$ signifies the symbol of Pochhammer.

Assuming that N is a positive integer, then the following three-term recurrence relations hold for $\{J_i^{p,q}(x)\}_{i=0}^N$, as they hold for all classical orthogonal polynomials

$$\begin{cases} J_0^{p,q}(x) = 1, \\ J_1^{p,q}(x) = \frac{1}{2}(2+p+q)x + \frac{1}{2}(p-q), \\ J_{i+1}^{p,q}(x) = (A_i^{p,q}x - B_i^{p,q})J_i^{p,q}(x) - C_i^{p,q}J_{i-1}^{p,q}(x), \ 1 \le i \le N. \end{cases}$$

$$(9)$$

where the coefficients of recursion are provided by

$$\begin{cases} A_i^{p,q} = \frac{(2i+p+q+1)(2i+p+q+2)}{2(i+1)(i+p+q+1)}, \\ B_i^{p,q} = \frac{(2i+p+q+1)(p^2-q^2)}{2(i+1)(i+p+q+1)(2i+p+q)}, \\ C_i^{p,q} = \frac{(2i+p+q+2)(i+p)(i+q)}{(i+1)(i+p+q+1)(2i+p+q)}. \end{cases}$$
(10)

The existence of orthogonality in the set of Jacobi polynomials is due to a weight function, which is represented by $\omega^{p,q}(x) = (1-x)^p (1+x)^q$, more precisely,

$$\int_{-1}^{1} J_{i}^{p,q}(x) J_{j}^{p,q}(x) \omega^{p,q}(t) dx = \iota_{i}^{p,q} \delta_{i,j}, \qquad (11)$$

where $\delta_{i,j}$ represents the function of the Kronecker delta, and

$$\iota_i^{p,q} = \frac{2^{(p+q+1)}\Gamma(i+p+1)\Gamma(i+q+1)}{(2i+p+q+1)i!\Gamma(i+p+q+1)}.$$
(12)

In specifically, the Legendre polynomial is a subclass of the Jacobi polynomial, which it can be stated as:

$$L_i(x) = J_i^{0,0}(x) = {}_2F_1\left(-i, i+1; 1; \frac{1-x}{2}\right).$$
(13)

0.3 Some auxiliary lemmas

Several important lemmas needed for theoretical investigation are summarized here. In what follows, C and C_{Φ} shall stand for positive constants that are not tied to the values of τ , N, and n and that may vary depending on the context. Additionally, we accept on the convention $\mathbb{Z}_{[a,b]} = \mathbb{Z} \cap [a,b]$, where \mathbb{Z} is the set of all positive integers. For the rest of this discussion, we'll be using the following notation

$$A(\Phi, w) = \kappa c_{\alpha} \left[\left({}_{a} D_{x}^{\alpha/2} \Phi, {}_{x} D_{b}^{\alpha/2} w \right) + \left({}_{x} D_{b}^{\alpha/2} \Phi, {}_{a} D_{x}^{\alpha/2} w \right) \right], \quad w \in \mathcal{W}_{N}^{0}.$$
(14)

The orthogonal projection operator, denoted by $\pi_N^{\frac{\alpha}{2},0}: H_0^{\frac{\alpha}{2}}(\Omega) \to \mathcal{W}_N^0$, will possess the following property:

$$A(\Phi - \pi_N^{\frac{\alpha}{2},0}\Phi, w) = 0, \quad \forall \Phi \in H_0^{\frac{\alpha}{2}}(\Omega), \quad w \in \mathcal{W}_N^0.$$
(15)

We provide the following semi-norm and norm to facilitate theoretical analysis.

$$|\Phi|_{\alpha/2} := A(\Phi, \Phi)^{1/2}, \tag{16}$$

$$\|\Phi\|_{\alpha/2} := (\|\Phi\|^2 + |\Phi|^2_{\alpha/2})^{1/2}.$$
(17)

Which are equivalent with the semi-norms and norms of $J_L^{\alpha/2}(\Omega), J_R^{\alpha/2}(\Omega), J_S^{\alpha/2}(\Omega)$ and $H^{\alpha/2}(\Omega)$. Next, we recall the following three lemmas from [118].

Lemma 0.2. Suppose that α and s are two real integers such that $\alpha \neq 1/2$, $0 < \alpha < 1$, $\alpha < s$. Then, for every function $\Phi \in H_0^{\frac{\alpha}{2}}(\Omega) \cap H^s(\Omega)$, the approximation that follows valid

$$|\Phi - \pi_N^{\frac{\alpha}{2},0} \Phi|_{\frac{\alpha}{2}} \le C N^{\frac{\alpha}{2}-s} \, \|\Phi\|_s \,, \tag{18}$$

where C is a positive constant C independent of N.

Lemma 0.3. We assume that $\Phi \in H_0^{\frac{\alpha}{2}}(\Omega)$ and that $\Omega = (a, b)$. Then, there are two positive, independent constants $C_1 < 1$ and C_2 with respect to Φ , such that the following remains true

$$C_1 \|\Phi\|_{\frac{\alpha}{2}} \le |\Phi|_{\frac{\alpha}{2}} \le \|\Phi\|_{\frac{\alpha}{2}} \le C_2 |\Phi|_{H^{\frac{\alpha}{2}}(\Omega)}.$$

Lemma 0.4. The inverse inequality that follows holds true for every given set of values for $\Phi \in \mathcal{P}_N(\Omega)$

$$\|\Phi\|_{\infty} \le CN \|\Phi\|, \tag{19}$$

where C is a constant that is positive and independent of Φ and N.

The properties of the interpolation operator I_N are summarized in the following lemma and remark.

Lemma 0.5 (see [119]). Assume that $\Phi \in H^s(\Omega)$, then for $s \ge 1$ and $0 \le l \le 1$, the following relation is valid

$$\left\|\Phi - I_N \Phi\right\|_l \le C N^{l-s} \left\|\Phi\right\|_s,$$

where C > 0 is a constant independent of N.

Remark 0.2 (see [91]). The smoothness of the solution to a fractional differential equation does not imply the smoothness of the source term. Consequently, the solution Φ has a different regularity order s than the regularity order r for the source term g, which means that

$$\|I_N g - g\| \le C N^{-r} \|\Phi\|_r, \quad \forall g \in H^r(\Omega),$$

where C > 0 is a constant independent of N, Φ and g.

Lemma 0.6 (see [120]). For any function $\Phi(t)$ which is absolutely continuous on [0, T], the following inequality is satisfied

$$\left(\frac{\partial^{\beta}}{\partial t^{\beta}}\Phi(t),\Phi(t)\right) \ge \frac{1}{2}\frac{\partial^{\beta}}{\partial t^{\beta}} \|\Phi(t)\|^{2}.$$
(20)

Definition 0.9 (L1 discrete time-fractional difference operator [91]). Let Φ^n , $0 \le n \le M$ be a given sequence of real functions such that M is is a positive integer, and let that the time interval is equally discretized by a time step τ , then we can define the L1 discrete time-fractional difference operator D^{β}_{τ} as follow

$$D_{\tau}^{\beta}\Phi^{n} = \frac{\tau^{-\beta}}{\Gamma(2-\beta)} \sum_{i=1}^{n} a_{n-i} \ \delta_{t}\Phi^{i} = \frac{\tau^{-\beta}}{\Gamma(2-\beta)} \sum_{i=0}^{n} b_{n-i}\Phi^{i}, \quad \forall n = 1, \dots, M.$$
(21)

In this expression, $\delta_t \Phi^i = \Phi^i - \Phi^{i-1}$, and the constants are defined by $b_0 = a_0$, $b_n = -a_{n-1}$, $b_{n-i} = a_{n-i} - a_{n-i-1}$, for each i = 1, ..., n-1.

Lemma 0.7 (see [77]). The discrete counterpart to the inequality (20) is given as

$$\left(D_{\tau}^{\beta}\Phi^{k}, \Phi^{k}\right) \geq \frac{1}{2}D_{\tau}^{\beta}\left\|\Phi^{k}\right\|^{2}, \quad \forall k = 1, \dots, M.$$

$$(22)$$

Next, we recall the $L2 - 1_{\sigma}$ discrete time-fractional difference operator [77].

Definition 0.10. The following coefficients are defined for any value of the parameter $\sigma = 1 - \frac{\beta}{2}$, $0 < \beta < 1$,

$$\mathcal{A}_{l}^{(\beta,\sigma)} = \begin{cases} \sigma^{1-\beta}, & l = 0, \\ (l+\sigma)^{1-\beta} - (l-1+\sigma)^{1-\beta}, & l \ge 1, \end{cases}$$
(23)

$$\mathcal{B}_{l}^{(\beta,\sigma)} = \frac{1}{2-\beta} \left[(l+\sigma)^{2-\beta} - (l-1+\sigma)^{2-\beta} \right] -\frac{1}{2} \left[(l+\sigma)^{1-\beta} + (l-1+\sigma)^{1-\beta} \right], \quad l \ge 1,$$
(24)

and

$$\mathcal{C}_{l}^{(k,\beta,\sigma)} = \begin{cases}
\mathcal{A}_{0}^{(\beta,\sigma)}, & l = k = 0, \\
\mathcal{A}_{0}^{(\beta,\sigma)} + \mathcal{B}_{1}^{(\beta,\sigma)}, & l = 0, k \ge 1, \\
\mathcal{A}_{l}^{(\beta,\sigma)} + \mathcal{B}_{l+1}^{(\beta,\sigma)} - \mathcal{B}_{l}^{(\beta,\sigma)}, & 1 \le l \le k - 1, \\
\mathcal{A}_{k}^{(\beta,\sigma)} - \mathcal{B}_{k}^{(\beta,\sigma)}, & 1 \le l = k.
\end{cases}$$
(25)

Consequently, the $L2-1_{\sigma}$ difference formula which applied in this investigation can be formulated in light of the lemma below.

Lemma 0.8. Under the premise that $\Phi(t) \in C^3[0, t_{k+1}], 0 \le k \le M - 1$, the high order $L2 - 1_{\sigma}$ difference formula reads as follows:

$${}_{0}D^{\beta}_{t_{k+\sigma}}\Phi = \frac{\tau^{-\beta}}{\Gamma(2-\beta)}\sum_{l=0}^{k} \mathcal{C}^{(k,\beta,\sigma)}_{k-l}\delta_{t}\Phi^{l} + O(\tau^{3-\beta}), \quad 0 < \beta < 1,$$
(26)

where $\delta_t \Phi^l = \Phi^{l+1} - \Phi^l$. For ease of theoretical analysis, we rewrite (26) in an equivalent form as

$${}_{0}D^{\beta}_{t_{k+\sigma}}\Phi = \frac{\tau^{-\beta}}{\Gamma(2-\beta)}\sum_{l=0}^{k}\mathcal{D}^{(k,\beta,\sigma)}_{l}\Phi^{l} + O(\tau^{3-\beta}), \qquad (27)$$

where $\mathcal{D}_1^{(0,\beta,\sigma)} = -\mathcal{D}_0^{(0,\beta,\sigma)} = \sigma^{1-\beta}$, for k = 0, and for $k \ge 1$,

$$\mathcal{D}_{l}^{(k,\beta,\sigma)} = \begin{cases} -\mathcal{C}_{k}^{(k,\beta,\sigma)}, & l = 0, \\ \mathcal{C}_{k-l+1}^{(k,\beta,\sigma)} - \mathcal{C}_{k-l}^{(k,\beta,\sigma)}, & 1 \le l \le k, \\ \mathcal{C}_{0}^{(k,\beta,\sigma)}, & l = k+1. \end{cases}$$
(28)

Definition 0.11 $(L2 - 1_{\sigma} \text{ discrete time-fractional difference operator}). Denote <math>t_{k+\sigma} = (k+\sigma)\tau = \sigma t_{k+1} + (1-\sigma)t_k$. For the temporal Caputo fractional derivative, the $L2 - 1_{\sigma}$ approximation formula at node $t_{k+\sigma}, k \in \mathbb{Z}_{[0,M-1]}$ is defined as

$${}_{0}D^{\beta}_{\tau}\Phi^{k+\sigma} = \frac{\tau^{-\beta}}{\Gamma(2-\beta)} \sum_{l=0}^{k+1} \mathcal{D}^{(k,\beta,\sigma)}_{l}\Phi^{l}, \quad 0 < \beta < 1.$$
(29)

Lemma 0.9 (see [77]). The following inequality holds for any $\Phi(t)$ identified on the interval Ω and $\beta \in (0,1)$. If $\Phi^{k+\sigma} = \sigma \Phi^{k+1} + (1-\sigma)\Phi^k$, then

$$\left(D_{\tau}^{\beta}, \Phi^{k+\sigma}\right) \geq \frac{1}{2} \left|D_{\tau}^{\beta}\right| \left|\Phi^{k+\sigma}\right|^{2}, \quad \forall k = 1, \dots, M.$$

By means of Taylor's theorem, it is observe that the following lemma is valid.

Lemma 0.10. (see [85]) For a given function $\Phi(t) \in C^2[0,T]$, the following identities hold

$$\Phi(\cdot, t_{k+\sigma}) = \sigma \ \Phi(\cdot, t_{k+1}) + (1 - \sigma) \ \Phi(\cdot, t_k) + O(\tau^2),
\Phi(\cdot, t_{k+\sigma}) = (\sigma + 1) \ \Phi(\cdot, t_k) - \sigma \ \Phi(\cdot, t_{k-1}) + O(\tau^2),
\Phi(\cdot, t_{k+\sigma-N_s}) = \sigma \ \Phi(\cdot, t_{k+1-N_s}) + (1 - \sigma) \ \Phi(\cdot, t_{k-N_s}) + O(\tau^2).$$
(30)

It's worth noting that a significant amount of consideration has been paid to developing fractional Grönwall inequalities in their continuous form in recent years. However, their discrete form has received less attention, and a few recent studies [82–84; 121] have attempted to close the gap. In what follows, we present a developed discrete versions of Grönwall inequality that agrees with the L1 and $L2-1_{\sigma}$ difference schemes and plays an important part in demonstrating the stability and convergence of the theoretical studies.

Lemma 0.11 (L1-Discrete fractional Grönwall inequality [84]). Assume that $\{\Phi^i\}_{i=-N_s}^{\infty}$ and $\{\zeta^n\}_{n=0}^{\infty}$ are both non-negative sequences. Suppose that $\mu_i, i \in \mathbb{Z}_{[1,4]}$

and c_0 are independent positive constants with respect to τ , such that the sequences satisfying

$$\begin{split} \Phi^{i} &\geq 0 \ for \ all \ i \geq 0, \ \Phi^{0} \ is \ known \ and \ \Phi^{i} = 0 \ if \ i < 0, \\ D^{\beta}_{\tau} \Phi^{j} &\leq \mu_{1} \Phi^{j} + c_{0} \zeta^{j}, \ \forall j \leq N_{s}, \\ D^{\beta}_{\tau} \Phi^{j} &\leq \mu_{1} \Phi^{j} + \mu_{2} \Phi^{j-1} + \mu_{3} \Phi^{j-2} + \mu_{4} \Phi^{j-N_{s}} + c_{0} \zeta^{j}, \ \forall j > N_{s}, \end{split}$$

then there exists a positive constant $\tau \leq \tau^* = \sqrt[\beta]{1/(2\Gamma(2-\beta)\mu_1)}$ such that

$$\Phi^{n} \leq 2 \left[\frac{c_0 t_n^{\beta}}{\Gamma(1+\beta)} \max_{0 \leq j \leq n} \zeta^j + \Phi^0 \right] E_{\beta}(2\mu t_n^{\beta}), \tag{31}$$

where $E_{\beta}(z) = \sum_{k=0}^{\infty} z^k / \Gamma(1+k\beta)$ is the Mittag-Leffler function and

$$\mu = \mu_1 + \frac{\mu_2}{a_0 - a_1} + \frac{\mu_3}{a_1 - a_2} + \frac{\mu_4}{a_{N_s - 1} - a_{N_s}}.$$
(32)

Lemma 0.12 $(L2-1_{\sigma} \text{ discrete fractional Grönwall inequality}[85; 86])$. Assume that $\{\Phi^i\}_{i=-N_s}^{\infty}$ and $\{\zeta^n\}_{n=0}^{\infty}$ are both non-negative sequences. Suppose that $\mu_i, i \in \mathbb{Z}_{[1,6]}$ are independent positive constants with respect to τ , such that for all $k \leq N_s$, the sequences satisfying

$$\begin{split} \Phi^{i} &\geq 0 \ \forall \ i \geq 0, \quad \Phi^{0} \ is \ known \ and \ \Phi^{i} = 0 \ \forall \ i < 0, \\ {}_{0}D^{\beta}_{t_{k+\sigma}} \Phi^{k} &\leq \mu_{1} \Phi^{k} + \zeta^{k}, \\ {}_{0}D^{\beta}_{t_{k+\sigma}} \Phi^{k} &\leq \mu_{1} \Phi^{k} + \mu_{2} \Phi^{k-1} + \mu_{3} \Phi^{k-2} + \mu_{4} \Phi^{k-3} + \mu_{5} \Phi^{k+1-N_{s}} + \mu_{6} \Phi^{k-N_{s}} + \zeta^{k}, \end{split}$$

in that case, there is a positive constant $\tau \leq \tau^* = \sqrt[\beta]{1/(2\Gamma(2-\beta)\mu_1)}$, which causes

$$\Phi^{k+1} \le 2E_{\beta}(2\mu t_k^{\beta}) \left(\Phi^0 + \frac{t_k^{\beta}}{\Gamma(1+\beta)} \max_{0 \le k_0 \le k} \zeta^{k_0} \right),$$

where $E_{\beta}(z)$ represent the Mittag-Leffler function and

$$\mu = \mu_1 + \frac{\mu_2}{b_0^{(\beta,\sigma)} - b_1^{(\beta,\sigma)}} + \frac{\mu_3}{b_1^{(\beta,\sigma)} - b_2^{(\beta,\sigma)}} + \frac{\mu_4}{b_2^{(\beta,\sigma)} - b_3^{(\beta,\sigma)}} + \frac{\mu_5}{b_{N_s-2}^{(\beta,\sigma)} - b_{N_s-1}^{(\beta,\sigma)}} + \frac{\mu_6}{b_{N_s-1}^{(\beta,\sigma)} - b_{N_s}^{(\beta,\sigma)}} + \frac{\mu_6}{b_{N_s-1}^{(\beta,\sigma)} - b_{N_s}^{(\beta,\sigma)} -$$

Chapter 1 Numerical method for the nonlinear time-space fractional reaction-diffusion equations with delay

In this chapter, we construct and analyze a linearized finite difference/Galerkin-Legendre spectral scheme for the nonlinear Riesz-space and Caputo-time fractional reaction-diffusion equation with time delay. The problem is first approximated by the L1 difference formula in the temporal direction, and then the Galerkin-Legendre spectral method is applied for the spatial discretization. The stability and the convergence of the semi-discrete approximation are proved by invoking the discrete fractional Halanay inequality. The stability and convergence of the fully discrete scheme are also investigated utilizing discrete fractional Grönwall inequalities, which show that the proposed method is stable and convergent. Furthermore, to verify the efficiency of our method, we provide numerical results that show a satisfactory agreement with the theoretical analysis.

1.1 Preliminary results and problem formulation

The literature has paid considerable attention to fractional partial differential equations involving delays. In what follows, we mention some of these works that relate to our problem under consideration. In [122], Lu developed a mono iterative scheme for the solution of the finite-difference system derived from a class of nonlinear delay reaction-diffusion systems. In [123], there is a consideration of an algorithm based on Legendre approximations for solving the fractional delay differential equations. Sun and Zhang in [124] used a linear compact difference scheme to solve the scalar delay parabolic equations. A spectrally accurate Petrov–Galerkin spectral scheme for fractional delay differential equations is developed in [125] by Zayernouri and his co-authors. This scheme is developed based on a new spectral theory for fractional Sturm–Liouville problems. The Chebyshev wavelet approach was suggested for the fractional delay differential equations by Saeed et al. in [126]. Liu and Zhang in [127] constructed a fully discrete scheme based on combining the Crank–Nicolson method and the Legendre spectral Galerkin method for the two-dimensional nonlinear delay diffusion-reaction equations. A numerical scheme for a class of non-linear time-delay fractional diffusion equations with distributed order in time was proposed in [128]. This study covers the unique solvability, convergence, and stability of the resulting numerical solution employing the discrete energy method. A numerical scheme for a class of non-linear distributed order fractional diffusion-wave equations with fixed time-delay is considered in [129]. The focus lies in the derivation of a linearized compact difference scheme as well as quantitatively analyzing it. Using the Lebesgue dominated convergence theorem, the Leray–Schauder fixed point theorem, and the Banach contraction mapping theorem, the authors in [130] obtain some sufficient conditions for the existence of the solutions of time Caputo fractional order partial differential equations with multi-delays. A linearized quasi-compact finite difference approach for semilinear space fractional diffusion equations with a fixed time delay was developed by Hao and colleagues [131]. It seems that theoretical analysis for that kind of problems is very rare. In spite of that, by using the semigroup theory of operators and the monotone iterative technique, the existence and uniqueness of mild solutions for the abstract time-space evolution equation with delay under some quasi-monotone conditions are obtained. The abstract results are applied to the time-space fractional delayed diffusion equation with fractional Laplacian operator, see [132].

This chapter is considered a continuation of the work [91], in which numerical and theoretical analysis were proposed for time and space fractional reaction-diffusion equations with respect to smooth and nonsmooth solutions. Both uniform and graded L1 schemes were invoked for that purpose side by side to Galerkin–Legendre spectral approximation of Legendre type. The main contribution of this chapter is to extend these numerical and theoretical results for time delay problems. That extension is not trivial due to the new challenges that appeared in the formulation of a linearized scheme and also in the theoretical analysis (convergence and stability) in the case of semi and fully-discrete schemes. The first challenge is solved in Section 1.3 by invoking the recent discrete inequalities of Halanay type and the second one is solved in Section 1.4 by recalling a suitable form of discrete fractional Grönwall inequalities which can deal with time delay functions. In light of these recent advances, we ponder conducting this case study. Without loss of generality, we consider the numerical approximations to the following nonlinear time-space fractional reaction-diffusion equations with delay

$$\frac{\partial^{\beta}\Phi}{\partial t^{\beta}} = \kappa \frac{\partial^{\alpha}\Phi}{\partial |x|^{\alpha}} + f(\Phi(x,t),\Phi(x,t-s)) + g(x,t), \quad x \in \Omega, \quad t \in I,$$
(1.1)

endowed with initial-boundary conditions of the form

$$\begin{cases} \Phi(x,t) = \psi(x,t), & x \in \Omega, \quad t \in [-s,0], \\ \Phi(a,t) = \Phi(b,t) = 0, \quad t \in I. \end{cases}$$
(1.2)

Here, $\Omega = [a, b] \subset \mathbb{R}$ and $I = [0,T] \subset \mathbb{R}$ are space and time domains, respectively. And $0 < \beta < 1$ is the time fractional order such that the time-fractional derivative is understood in the sense of Caputo. The positive constants κ , and s, denote the diffusion and temporal delay parameters, respectively. Also, $1 < \alpha < 2$ is the space fractional order.

1.2 Derivation of Numerical Scheme

This section is devoted to constructing a fully discrete scheme for the problem (1.1)-(1.2), based on combining L1 approximation formula and the Legendre-Galerkin spectral method in order to discretize the temporal and space-fractional derivatives, respectively. We begin with temporal discretization and then detail the suggested scheme's spatial discretization.

1.2.1 Temporal discretization

We choose a time step given by $\tau = \frac{s}{N_s}$, where N_s is a positive integer, in order to uniformly divide the temporal domain I. This defines a class of uniform partitions denote by $t_n = n\tau$, for each $-N_s \leq n \leq M$, where $M = \left\lceil \frac{T}{\tau} \right\rceil$. Denote $\Phi^n = \Phi(., t_n)$, then the following expressions can be used to get the L1 estimate for the Caputo-time fractional derivative (6) of order $0 < \beta < 1$ at the time t_n , as [91]

$$\frac{\partial^{\beta} \Phi(x,t)}{\partial t^{\beta}}\Big|_{t=t_{n}} = \int_{0}^{t_{n}} \Phi'(x,\eta) \omega_{1-\beta}(t_{n}-\eta) d\eta
= \frac{1}{\Gamma(1-\beta)} \sum_{i=1}^{n} \frac{\Phi(x,t_{i}) - \Phi(x,t_{i-1})}{\tau} \int_{t_{i-1}}^{t_{i}} (t_{n}-\eta)^{-\beta} d\eta + r_{\tau}^{n}
= \frac{1}{\tau^{\beta} \Gamma(2-\beta)} \sum_{i=1}^{n} a_{n-i} \left(\Phi(x,t_{i}) - \Phi(x,t_{i-1})\right) + r_{\tau}^{n}
= D_{\tau}^{\beta} \Phi^{n} + r_{\tau}^{n},$$
(1.3)

where D_{τ}^{β} is the L1 discrete time-fractional difference operator given by (21), and the kernel $\omega_{\beta}(t) = \frac{t^{\beta-1}}{\Gamma(\beta)}$, for all t > 0. Also, for each $j \ge 0$ the coefficients a_j satisfy $a_j = (j+1)^{1-\beta} - j^{1-\beta}$. For each $n = 0, 1, \ldots, M$, if the function $\Phi \in C^2([0,T]; L^2(\Omega))$, then there is a positive constant C > 0 which means that the truncation error meets $||r_{\tau}^n|| \le C\tau^{2-\beta}$, (see [68]).

Following that, at each time t_n , we shall present a semi-discretized version of (1.1)-(1.2). To this end, the uniform formula (21) is used to estimate the time-fractional component, and Taylor's approximations are used to discretize the nonlinear source term. Thus, the resulting discrete-time system is as follows:

$$\begin{cases} D^{\beta}_{\tau}\Phi^{n} = \frac{\partial^{\alpha}\Phi^{n}}{\partial|x|^{\alpha}} + f(2\Phi^{n-1} - \Phi^{n-2}, \Phi^{n-N_{s}}) + g^{n}(x), & 1 \le n \le M, \quad x \in \Omega, \\ \Phi^{n}(x) = \psi(x), & -N_{s} \le n \le 0, \quad x \in \Omega, \end{cases}$$
(1.4)

Let us consider the coefficient $\lambda := \Gamma(2-\beta)\tau^{\beta}$. Then the semi-scheme (1.4) can be rewritten in the following equivalent form:

$$\Phi^{n} - \lambda \kappa \frac{\partial^{\alpha} \Phi^{n}}{\partial |x|^{\alpha}} = a_{n-1} \Phi^{0} - \sum_{i=1}^{n-1} b_{n-i} \Phi^{i} + \lambda f (2\Phi^{n-1} - \Phi^{n-2}, \Phi^{n-N_s})$$
$$+ \lambda g^{n}(x), \quad \forall n = 1, \dots, M.$$
(1.5)

1.2.2 Spatial discretization

We first present the space function below to give suitable base functions that precisely meet the boundary requirements specified in spectral techniques for space-fractional differential equations in order to discretize the space-fractional derivatives [118; 133]:

$$\mathcal{W}_N^0 = \mathcal{P}_N(\Omega) \cap H_0^1(\Omega) = \operatorname{span} \left\{ \varphi_n(x) : n = 0, 1, \dots, N - 2 \right\}.$$
(1.6)

For this purpose, we introduce the following rescale functions [94]:

$$\wedge : [a,b] \mapsto [-1,1] : x \mapsto \frac{2x - (a+b)}{(b-a)};$$

$$\wedge^{-1} : [-1,1] \mapsto [a,b] : t \mapsto \frac{(b-a)t + a + b}{2}.$$

By acting $\wedge(x)$ as \hat{x} , then the basis functions φ_n chosen for the spatial discretization can be given for each $\hat{x} \in [-1, 1]$, as

$$\varphi_n(x) = L_n(\hat{x}) - L_{n+2}(\hat{x}) = \frac{2n+3}{2(n+1)}(1-\hat{x}^2)J_n^{1,1}(\hat{x}), \quad (1.7)$$

with $x = \frac{1}{2}((b-a)\hat{x} + a + b) \in [a, b]$. Hence, the fully discrete L1-Galerkin spectral scheme for the problem (1.1)-(1.2) consists of the set of approximations $\Phi_N^n \in \mathcal{W}_N^0$, satisfying the following system

$$\begin{cases} (\Phi_N^n, \upsilon) - \lambda \left(\frac{\partial^{\alpha}}{\partial |x|^{\alpha}} \Phi_N^n, \upsilon \right) = a_{n-1} \left(\Phi_N^0, \upsilon \right) - \sum_{i=1}^{n-1} b_{n-i} \left(\Phi_N^i, \upsilon \right) \\ + \lambda \left(I_N f(2\Phi_N^{n-1} - \Phi_N^{n-2}, \Phi_N^{n-N_s}), \upsilon \right) + \lambda \left(I_N g^n(x), \upsilon \right), \ \forall \upsilon \in \mathcal{W}_N^0, \ \forall n = 1, \dots, M, \\ \Phi_N^n = \pi_N^{1,0} \psi(t_n, x), \quad -N_s \le n \le 0, \end{cases}$$

$$(1.8)$$

where $\pi_N^{1,0}$ is a suitable projection operator in this case. Following this, we expand the approximate solutions as

$$\Phi_N^n = \sum_{i=0}^{N-2} \hat{\Phi}_i^n \varphi_i(x), \qquad (1.9)$$

where $\hat{\Phi}_i^n$ are the unknown expansion coefficients to be specified. The uniform full discrete scheme for the model (1.1)-(1.2) can be expressed as a linear system in a matrix form using (1.9), lemma 0.1 and allowing $v = \varphi_k$, for each $0 \le k \le N - 2$ as follows:

$$\left(\bar{M} - \lambda c_{\alpha}(S + S^{T})\right)U^{n} = K^{n-1} + \lambda H^{n-1} + \lambda G^{n}.$$
(1.10)

The notations in this expression are given by the system of identities

$$\begin{cases} s_{ij} = \int_{\Omega} {}_{a} D_{x}^{\frac{\alpha}{2}} \varphi_{i}(x)_{x} D_{b}^{\frac{\alpha}{2}} \varphi_{j}(x) dx, & S = (s_{ij})_{i,j=0}^{N-2}, \\ m_{ij} = \int_{\Omega} \varphi_{i}(x) \varphi_{j}(x) dx, & \bar{M} = (m_{ij})_{i,j=0}^{N-2}, \\ h_{i}^{n-1} = \int_{\Omega} \varphi_{i}(x) I_{N} f(2\Phi_{N}^{n-1} - \Phi_{N}^{n-2}, \Phi_{N}^{n-N_{s}}) dx, & H^{n-1} = (h_{0}^{n-1}, h_{1}^{n-1}, \dots, h_{N-2}^{n-1})^{\top}, \\ g_{i}^{n} = \int_{\Omega} \varphi_{i}(x) I_{N} g^{n} dx, & G^{n} = (g_{0}^{n}, g_{1}^{n}, \dots, g_{N-2}^{n})^{\top}, \\ U^{n} = (\hat{\Phi}_{0}^{n}, \hat{\Phi}_{1}^{n}, \dots, \hat{\Phi}_{N-2}^{n})^{\top}, & K^{n-1} = -\sum_{j=0}^{n-1} b_{n-j} \bar{M} U^{j}. \end{cases}$$

$$(1.11)$$

The elements of the stiffness matrix S and the mass matrix \overline{M} can easily handled using the following lemma.

Lemma 1.1 (see [118; 133]). The following relation can be used to manipulate the components that make up the stiffness matrix S, namely,

$$s_{ij} = a_i^j - a_i^{j+2} - a_{i+2}^j + a_{i+2}^{j+2}, \quad i, j = 0, 1, \dots, N-2,$$

where the coefficients a_i^j can be calculated as follows

$$a_{i}^{j} = \int_{\Omega} {}_{a} D_{x}^{\frac{\alpha}{2}} L_{i}(\hat{x})_{x} D_{b}^{\frac{\alpha}{2}} L_{j}(\hat{x}) dx$$

$$= \left(\frac{b-a}{2}\right)^{1-\alpha} \frac{\Gamma(i+1)\Gamma(j+1)}{\Gamma(i-\frac{\alpha}{2}+1)\Gamma(j-\frac{\alpha}{2}+1)} \cdot (1.12)$$

$$\cdot \sum_{r=0}^{N} \varpi_{r}^{-\frac{\alpha}{2},-\frac{\alpha}{2}} J_{i}^{\frac{\alpha}{2},-\frac{\alpha}{2}} \left(x_{r}^{-\frac{\alpha}{2},-\frac{\alpha}{2}}\right) J_{j}^{-\frac{\alpha}{2},\frac{\alpha}{2}} \left(x_{r}^{-\frac{\alpha}{2},-\frac{\alpha}{2}}\right),$$

and $\left\{\varpi_r^{-\frac{\alpha}{2},-\frac{\alpha}{2}}, x_r^{-\frac{\alpha}{2},-\frac{\alpha}{2}}\right\}_{i=0}^N$ is Jacobi-Gauss collection points and their corresponding weights related to the weight function $\omega^{-\frac{\alpha}{2},-\frac{\alpha}{2}}$. Additionally, the nonzero components

of the symmetric mass matrix \overline{M} are given by

$$m_{ij} = m_{ji} = \begin{cases} \frac{b-a}{2j+1} + \frac{b-a}{2j+5}, & \forall i = j, \\ -\frac{b-a}{2j+5}, & \forall i = j+2. \end{cases}$$
(1.13)

1.3 Theoretical analysis of the semi-discrete scheme

This section aims to investigate the effectiveness of the semi-discrete Galerkin spectral approaches for the (1.1). In turn, the semi-discrete Galerkin spectral scheme which is time continuous consists of the set of approximations $\Phi_N \in \mathcal{W}_N^0$, satisfying the system

$$\begin{cases} \left(\frac{\partial^{\beta}\Phi_{N}}{\partial t^{\beta}},\upsilon\right) - \left(\frac{\partial^{\alpha}}{\partial|x|^{\alpha}}\Phi_{N},\upsilon\right) \\ = \left(I_{N}f(\Phi_{N},\Phi_{N}(t-s)),\upsilon\right) + \left(I_{N}g_{N}(t),\upsilon\right), \quad \forall \upsilon \in \mathcal{W}_{N}^{0}, \ t \in I, \end{cases}$$

$$\Phi_{N}(t) = \pi_{N}^{1,0}\psi_{N}(t), \ t \in [-s,0], \qquad (1.14)$$

we make the assumptions that the delay $s = t - \vartheta_1 \ge \vartheta_0 > 0$ to avoid the possible clustering of discontinuous points due to vanishing delay [134]. We assume that Φ_N is the solution of the following week formulation of the semi-discrete scheme (1.14):

$$\begin{pmatrix} \frac{\partial^{\beta}}{\partial t^{\beta}} \Phi_N, \upsilon_N \end{pmatrix} + A(\Phi_N, \upsilon_N) = (I_N f(\Phi_N, \Phi_N(t-s)), \upsilon_N) + (I_N g_N(t), \upsilon_N), \quad \forall \upsilon \in \mathcal{W}_N^0, \quad t \in I, \quad (1.15)$$

with initial conditions

$$\Phi_N = \pi_N^{1,0} \phi_N(t), \quad t \in [-s,0].$$

We assume also that the problem (1.15) satisfies the one-sided Lipschitz condition

$$2(f(\Phi_1,\psi(\cdot)) - f(\Phi_2,\psi(\cdot)), \Phi_1 - \Phi_2) \le c \|\Phi_1 - \Phi_2\|^2, \qquad (1.16)$$

and the condition of Lipschitz

$$2(f(\Phi,\psi_1(\cdot)) - f(\Phi,\psi_2(\cdot)), \Phi_1 - \Phi_2) \le d \max_{t-\vartheta_2 \le \xi \le t-\vartheta_1} \|\Psi_1(\xi) - \Psi_2(\xi)\|^2, \quad (1.17)$$

for the continuous mapping f. Where $\Psi(\cdot) = \Phi(t-s)$, the constants c and d satisfy that $d \ge 0$ and c + d < 0, and the functions ϑ_1 , ϑ_2 also stay in the range such that $0 < \vartheta_0 \le \vartheta_1 \le \vartheta_2 \le t + s$. Now, we recall the following lemma which will be helpful in the coming analysis.

Lemma 1.2 (Fractional Halanay inequality [135]). Assume that the non-negative continuous function $\Phi(t)$ satisfies that

$$\begin{cases} \frac{\partial^{\beta}}{\partial t^{\beta}} \Phi(t) \leq \gamma + a \Phi(t) + b \max_{t-s \leq \xi \leq t} \Phi(\xi), & t \in I, \\ \Phi(t) = |\psi(t)|, & t \in [-s, 0], \end{cases}$$

where the constants γ , $b \ge 0$, a + b < 0, and the delay parameter $s \ge \vartheta_0 > 0$. Then the following estimate holds

$$\Phi(t) \le \frac{-\gamma}{a+b} + M E_{\beta}(\theta^* t^{\beta}), \qquad (1.18)$$

where $M = \max_{t \in [-s,0]} |\psi(t)|$, and the parameter θ^* is given as

$$\theta^* = \sup_{t-s \ge 1} \{\theta : \theta - a - b \left(E_\beta \left(\theta (t-s)^\beta \right) / E_\beta (\theta t^\beta) \right) = 0 \},$$
(1.19)

is strictly negative and the estimate in (1.18) holds for all t such that $t \ge s + 1$.

1.3.1 Stability

As a consequence of the previous lemma, we can state and prove the stability of the semi discrete scheme (1.15). Assume that $\tilde{\Phi}_N$ is the solution of

$$\begin{pmatrix} \frac{\partial^{\beta}}{\partial t^{\beta}} \tilde{\Phi}_{N}, \upsilon_{N} \end{pmatrix} + A \left(\tilde{\Phi}_{N}, \upsilon_{N} \right)$$

= $\left(I_{N} f \left(\tilde{\Phi}_{N}, \tilde{\Phi}_{N}(t-s) \right), \upsilon_{N} \right) + \left(I_{N} \tilde{g}_{N}(t), \upsilon_{N} \right), \quad \forall \upsilon \in \mathcal{W}_{N}^{0}, \quad t \in I, \quad (1.20)$

with initial conditions

$$\tilde{\Phi}_N = \pi_N^{1,0} \phi_N(t), \quad t \in [-s,0].$$

Theorem 1.1. The semi-discrete scheme (1.15) induced by the two assumptions (1.16) and (1.17) is stable in the sense that for all $\tau > 0$, it holds

$$\left\|\Phi_N - \tilde{\Phi}_N\right\|^2 \le C.$$

where C is a positive constant independent of N.

Proof. Denote $\rho_N = \Phi_N - \tilde{\Phi}_N$. Subtracting (1.20) from (1.15), it holds

$$\begin{pmatrix} \frac{\partial^{\beta}}{\partial t^{\beta}} \rho_N, \upsilon_N \end{pmatrix} + A(\rho_N, \upsilon_N)$$

= $\left(I_N f(\Phi_N, \Phi_N(t-s)) - I_N f(\tilde{\Phi}_N, \tilde{\Phi}_N(t-s)), \upsilon_N \right) + \left(I_N g_N(t) - I_N \tilde{g}_N(t), \upsilon_N \right).$ (1.21)

Taking $v_N = \rho_N$. Invoking (1.16) and (1.17) and using Triangle inequality, Hölder inequality and Young's inequality, we derive that for the first term of the right hand side

$$\begin{split} &\left(I_N f(\Phi_N, \Phi_N(t-s)) - I_N f(\tilde{\Phi}_N, \tilde{\Phi}_N(t-s)), \rho_N\right) \\ &= \left(I_N f(\Phi_N, \Phi_N(t-s)) - I_N f(\Phi_N, \tilde{\Phi}_N(t-s)), \rho_N\right) \\ &+ \left(I_N f(\Phi_N, \tilde{\Phi}_N(t-s)) - I_N f(\tilde{\Phi}_N, \tilde{\Phi}_N(t-s)), \rho_N\right) \\ &\leq \frac{d}{2} C \max_{t-\vartheta_2 \leq \xi \leq t-\vartheta_1} \left\|\Psi(\xi) - \tilde{\Psi}(\xi)\right\| \left\|\Psi(t) - \tilde{\Psi}(t)\right\| + \frac{c}{2} \|\rho_N\|^2 \\ &\leq \frac{d}{2} C \max_{t-\vartheta_2 \leq \xi \leq t} \left\|\Psi(\xi) - \tilde{\Psi}(\xi)\right\| \left\|\Psi(t) - \tilde{\Psi}(t)\right\| + \frac{c}{2} \|\rho_N\|^2 \\ &\leq \frac{d}{2} C \max_{t-\vartheta_2 \leq \xi \leq t} \left\|\Psi(\xi) - \tilde{\Psi}(\xi)\right\|^2 + \frac{c}{2} \|\rho_N\|^2 \,, \end{split}$$

and for the second term

$$(I_N g_N(t) - I_N \tilde{g}_N(t), \rho_N) \le \frac{\epsilon}{2} C \|g_N(t) - \tilde{g}_N(t)\|^2 + \frac{1}{2\epsilon} \|\rho_N\|^2.$$

Then (1.21) becomes

$$\left(\frac{\partial^{\beta}}{\partial t^{\beta}}\rho_{N}, \rho_{N}\right) + A\left(\rho_{N}, \rho_{N}\right)$$

$$\leq \left(\frac{c}{2} + \frac{1}{2\epsilon}\right) \left\|\rho_{N}\right\|^{2} + \frac{d}{2}C \max_{t-\vartheta_{2} \leq \xi \leq t} \left\|\Psi(\xi) - \tilde{\Psi}(\xi)\right\|^{2} + \frac{\epsilon}{2}C \left\|g_{N}(t) - \tilde{g}_{N}(t)\right\|^{2}.$$

Using (20) and (16), we can deduce that

$$\frac{1}{2} \frac{\partial^{\beta}}{\partial t^{\beta}} \left\| \rho_{N}^{k} \right\|^{2} + \left| \rho \right|_{\alpha/2}^{2} \\ \leq \left(\frac{c}{2} + \frac{1}{2\epsilon} \right) \left\| \rho_{N} \right\|^{2} + \frac{d}{2} C \max_{t - \vartheta_{2} \le \xi \le t} \left\| \Psi(\xi) - \tilde{\Psi}(\xi) \right\|^{2} + \frac{\epsilon}{2} C \left\| g_{N}(t) - \tilde{g}_{N}(t) \right\|^{2},$$

namely,

$$\frac{\partial^{\beta}}{\partial t^{\beta}} \|\rho_{N}\|^{2} \leq \left(c + \frac{1}{\epsilon}\right) \|\rho_{N}\|^{2} + dC \max_{t - \vartheta_{2} \leq \xi \leq t} \left\|\Psi(\xi) - \tilde{\Psi}(\xi)\right\|^{2} + \epsilon C \max_{t \in I} \left\|g_{N}(t) - \tilde{g}_{N}(t)\right\|^{2}.$$

By means of Lemma 1.2 and $\epsilon > 0$ is chosen to gurantee that $(c + 1/\epsilon) + dC < 0$, we have

$$\|\rho_N\|^2 \le \frac{-\gamma^*}{\left(c+\frac{1}{\epsilon}\right)+dC} + M^* E_\beta(\theta^{**} t^\beta), \qquad (1.22)$$

where $\gamma^* = \epsilon C \max_{t \in I} \|g_N(t) - \tilde{g}_N(t)\|^2$, $M^* = \max_{\xi \in [-s,0]} \|\pi_N^{1,0} \psi_N(\xi) - \pi_N^{1,0} \phi_N(\xi)\|^2$, and the parameter θ^{**} is given as

$$\theta^{**} = \sup_{t-\vartheta_2 \ge 1} \{\theta : \theta - (c+1/\epsilon) - dC \left(E_\beta \left(\theta(t-\vartheta_2)^\beta \right) / E_\beta(\theta t^\beta) \right) = 0 \}, \quad (1.23)$$

is strictly negative and the estimate in (1.22) holds for all t such that $t \ge \vartheta_2 + 1$. \Box

1.3.2 Convergence

In this subsection, we investigate the convergence of semi-discrete scheme (1.15) using error estimation.
Theorem 1.2. Assume that $\Phi \in C^{0,\alpha}([0,T], H^s(\Omega))$ with respect to $D_t^{\alpha}\Phi \in C\left([0,T], H_0^{\frac{\alpha}{2}}(\Omega) \cap H^s(\Omega)\right)$ is the exact solution to problem (1.1)-(1.2) with $\psi \in C\left([-s,0], H^s(\Omega)\right)$ and suppose also Φ_N the solution of (1.15). Then for a positive constant C independent of N, the following statement is valid

$$|\Phi - \Phi_N|_{\alpha/2} \le C\left(N^{\alpha/2-s} + N^{-r}\right). \tag{1.24}$$

Proof. Denote $\Phi - \Phi_N = e_N = (\Phi - \pi_N^{\frac{\alpha}{2},0} \Phi) + (\pi_N^{\frac{\alpha}{2},0} \Phi - \Phi_N) \stackrel{\Delta}{=} \tilde{e}_N + \hat{e}_N$. The weak formulation of equation (1.1) is

$$(D_t^{\beta}\Phi, v_N) + A(\Phi, v_N) = (f(\Phi, \Phi(t-s)), v_N) + (g, v_N).$$
(1.25)

Subtracting (1.15) from (1.25) and owing to the definition of orthogonal projection, the error equation satisfies

$$(D_t^{\beta} e_N, \upsilon_N) + A(e_N, \upsilon_N) \stackrel{\Delta}{=} \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3, \qquad (1.26)$$

where

$$\mathcal{E}_{1} = (I_{N}f(\Phi, \Phi(t-s)) - I_{N}f(\Phi_{N}, \Phi_{N}(t-s)), \upsilon_{N}), \\ \mathcal{E}_{2} = (f(\Phi, \Phi(t-s)) - I_{N}f(\Phi, \Phi(t-s)), \upsilon_{N}), \\ \mathcal{E}_{3} = (g - I_{N}g, \upsilon_{N}).$$

We next estimate the right-hand terms \mathcal{E}_1 , \mathcal{E}_2 and \mathcal{E}_3 . For the first term \mathcal{E}_1 , by the aid of (1.16) and (1.17), and by taking $v_N = e_N$, we can deduce that

$$\mathcal{E}_{1} \leq \frac{d}{2} C \max_{t-\vartheta_{2} \leq \xi \leq t} \left\| \Psi(\xi) - \tilde{\Psi}(\xi) \right\|^{2} + \frac{c}{2} \left\| \hat{e}_{N} \right\|^{2} + \frac{c}{2} \left\| \tilde{e}_{N} \right\|^{2}, \qquad (1.27)$$

moreover, owing to Lemmas 0.2 and 0.3, it holds

$$\|\tilde{e}_N\|^2 \le \frac{C}{C_1} N^{\alpha - 2s} \|\Phi\|_s^2,$$

then (1.27) becomes

$$\mathcal{E}_{1} \leq \frac{d}{2} C \max_{t-\vartheta_{2} \leq \xi \leq t} \left\| \Psi(\xi) - \tilde{\Psi}(\xi) \right\|^{2} + \frac{c}{2} \left\| \hat{e}_{N} \right\|^{2} + \frac{c}{2} \frac{C}{C_{1}} N^{\alpha-2s} \left\| \Phi \right\|_{s}^{2}, \qquad (1.28)$$

For the second term \mathcal{E}_2 , by means of Lemma 0.5 and Hölder inequality, it holds

$$\mathcal{E}_{2} \leq \frac{\epsilon}{2} C N^{\alpha - 2s} \|\Phi\|_{L^{\infty}(-s,T;H^{s}(\Omega))}^{2} + \frac{1}{2\epsilon} \|\hat{e}_{N}\|^{2} + \frac{1}{2\epsilon} \frac{C}{C_{1}} N^{\alpha - 2s} \|\Phi\|_{s}^{2}.$$
(1.29)

For the third term R_3 , it holds by invoking Remark 0.2

$$\mathcal{E}_{3} \leq \frac{\epsilon}{2} C N^{\alpha - 2r} \|\Phi\|_{L^{\infty}(-s,T;H^{r}(\Omega))}^{2} + \frac{1}{2\epsilon} \|\hat{e}_{N}\|^{2} + \frac{1}{2\epsilon} \frac{C}{C_{1}} N^{\alpha - 2s} \|\Phi\|_{s}^{2}.$$
(1.30)

Substituting (1.28), (1.29), and (1.30) into (1.26), considering $v_N = e_N$ and invoking relation (20), we can infer that

$$D_{t}^{\beta} \|\hat{e}_{N}\|^{2} + 2|e_{N}|_{\alpha/2}^{2}$$

$$\leq 2(c/2 + 1/\epsilon) \|\hat{e}_{N}\|^{2} + dC \max_{t-\mu_{2} \leq \xi \leq t} \left\|\Psi(\xi) - \tilde{\Psi}(\xi)\right\|^{2} + \tilde{\mathcal{Q}}, \qquad (1.31)$$

where

$$\begin{split} \tilde{\mathcal{Q}} &= \epsilon \tilde{C} N^{\alpha - 2s} \left(\left| D_t^{\beta} \| \Phi \|_{L^{\infty}(0,T;H^s(\Omega))}^2 \right| + \left\| D_t^{\beta} \Phi \right\|_{L^{\infty}(0,T;H^s(\Omega))}^2 + \| \Phi \|_{L^{\infty}(-s,T;H^s(\Omega))}^2 \right) \\ &+ \epsilon \tilde{C} N^{-2r} \| \Phi \|_{L^{\infty}(-s,T;H^r(\Omega))}^2 \,. \end{split}$$

namely,

$$D_t^{\beta} \|\hat{e}_N\|^2 \le 2(c/2 + 1/\epsilon) \|\hat{e}_N\|^2 + dC \max_{t - \vartheta_2 \le \xi \le t} \left\|\Psi(\xi) - \tilde{\Psi}(\xi)\right\|^2 + \tilde{\mathcal{Q}},$$

by means of Lemma 1.2 and $\epsilon > 0$ is chosen to guarantee that $(c+2/\epsilon)+dC < 0$, we can complete as in Theorem.1.1. Finally, utilizing triangle inequality and Lemma 0.2, the proof is fulfilled.

1.4 Theoretical analysis of the fully discrete scheme

The purpose of this section is to study the efficiency of the fully discrete Galerkin spectral methods for the (1.1)-(1.2). We start by stability analysis and gives theorem of stability in the first subsection. The second subsection is devoted

to the convergence analysis and the theorem of convergence is given there. For the theoretical analysis requirements, we assume that the function f satisfies the following Lipschitz condition

$$|f(\Phi_1, v_1) - f(\Phi_2, v_2)| \le L \left(|\Phi_1 - \Phi_2| + |v_1 - v_2| \right), \tag{1.32}$$

where L is a positive constant.

1.4.1 Stability analysis

The weak formulation of the proposed scheme is as follows: find $\{\Phi_N^k\}_{k=1}^M \in \mathcal{P}_N$, such that satisfying the following

$$\left(D^{\beta}_{\tau} \Phi^{k}_{N}, \upsilon_{N} \right) + A \left(\Phi^{k}_{N}, \upsilon_{N} \right)$$

$$= \left(I_{N} f (2 \Phi^{k-1}_{N} - \Phi^{k-2}_{N}, \Phi^{k-N_{s}}_{N}), \upsilon_{N} \right) + \left(I_{N} g^{k}, \upsilon_{N} \right), \quad \forall \upsilon_{N} \in \mathcal{P}_{N},$$

$$(1.33)$$

with

$$\Phi_N^k = \pi_N^{1,0} \varphi^k, \ -N_s \le k \le 0.$$

It is a linear iterative scheme which means that we need only to get a solution to a system of linear equations at each time level. The well-posedness of the proposed scheme, that is, its unique solvability and continuous dependency on the initial-boundary conditions, is sufficient to validate the hypotheses of the well-known Lax– Milgram's lemma [136]. More specifically, in terms of (1.33), we see that the bilinear form $A(\cdot, \cdot)$ is continuous and coercive in $H_0^{\alpha/2} \times H_0^{\alpha/2}$. Assume that $\{\tilde{\Phi}_N^k\}_{k=1}^M$ is the solution of

$$\left(D_{\tau}^{\beta} \tilde{\Phi}_{N}^{k}, \upsilon_{N} \right) + A \left(\tilde{\Phi}_{N}^{k}, \upsilon_{N} \right)$$

$$= \left(I_{N} f (2 \tilde{\Phi}_{N}^{k-1} - \tilde{\Phi}_{N}^{k-2}, \tilde{\Phi}_{N}^{k-N_{s}}), \upsilon_{N} \right) + \left(I_{N} \tilde{g}^{k}, \upsilon_{N} \right), \quad \forall \upsilon_{N} \in \mathcal{P}_{N}$$

$$(1.34)$$

with initial conditions

$$\tilde{\Phi}_N^k = \pi_N^{1,0} \varphi^k, \quad -N_{\mathbf{s}} \le k \le 0.$$

Now, we present the theorem of stability in the following context.

Theorem 1.3. The fully discrete scheme (1.33) is unconditionally stable in the sense that for all $\tau > 0$, it holds

$$\left\|\Phi_N^k - \tilde{\Phi}_N^k\right\|^2 \le C \max_{1 \le k \le M} \left\|g^k - \tilde{g}^k\right\|^2.$$

Proof. Denote $\rho_N^k = \Phi_N^k - \tilde{\Phi}_N^k$. Subtracting (1.34) from (1.33), it holds

$$\begin{pmatrix} D_{\tau}^{\beta} \rho_{N}^{k}, \upsilon_{N} \end{pmatrix} + A \left(\rho_{N}^{k}, \upsilon_{N} \right)$$

$$= \left(I_{N} f \left(2\Phi_{N}^{k-1} - \Phi_{N}^{k-2}, \Phi_{N}^{k-N_{s}} \right) - I_{N} f \left(2\tilde{\Phi}_{N}^{k-1} - \tilde{\Phi}_{N}^{k-2}, \tilde{\Phi}_{N}^{k-N_{s}} \right), \upsilon_{N} \right)$$

$$+ \left(I_{N} g^{k} - I_{N} \tilde{g}^{k}, \upsilon_{N} \right).$$

$$(1.35)$$

According to (1.32) and using Hölder inequality and Young's inequality, we derive that for the first term

$$\left(I_N f(2\Phi_N^{k-1} - \Phi_N^{k-2}, \Phi_N^{k-N_s}) - I_N f(2\tilde{\Phi}_N^{k-1} - \tilde{\Phi}_N^{k-2}, \tilde{\Phi}_N^{k-N_s}), \upsilon_N \right)$$

$$\leq C L \left(\left\| 2\rho_N^{k-1} - \rho_N^{k-2} \right\| + \left\| \rho_N^{k-N_s} \right\| \right) \|\upsilon_N\|$$

$$\leq \frac{\epsilon}{2} C L^2 \left\| 2\rho_N^{k-1} - \rho_N^{k-2} \right\|^2 + \frac{\epsilon}{2} C L^2 \left\| \rho_N^{k-N_s} \right\|^2 + \frac{1}{2\epsilon} \|\upsilon_N\|^2$$

$$\leq 4\epsilon C L^2 \left\| \rho_N^{k-1} \right\|^2 + \epsilon L^2 \left\| \rho_N^{k-2} \right\|^2 + \frac{\epsilon}{2} C L^2 \left\| \rho_N^{k-N_s} \right\|^2 + \frac{1}{2\epsilon} \|\upsilon_N\|^2 ,$$

and for the second term

$$(I_N g^k - I_N \tilde{g}^k, v_N) \le \frac{\epsilon}{2} C \|g^k - \tilde{g}^k\|^2 + \frac{1}{2\epsilon} \|v_N\|^2.$$

Then (1.35) becomes

$$(D_{\tau}^{\beta}\rho_{N}^{k}, \upsilon_{N}) + A(\rho_{N}^{k}, \upsilon_{N})$$

$$\leq \frac{1}{\epsilon} \|\upsilon_{N}\|^{2} + 4\epsilon CL^{2} \|\rho_{N}^{k-1}\|^{2} + \epsilon L^{2} \|\rho_{N}^{k-2}\|^{2} + \frac{\epsilon}{2} CL^{2} \|\rho_{N}^{k-N_{s}}\|^{2} + \frac{\epsilon C}{2} \|g^{k} - \tilde{g}^{k}\|^{2}.$$

Taking $v_N = \rho_N^k$ and using (22) and (16), we can deduce that

$$\frac{1}{2}D_{\tau}^{\beta} \left\|\rho_{N}^{k}\right\|^{2} + \left|\rho\right|_{\alpha/2}^{2} \leq \frac{1}{\epsilon} \left\|\rho_{N}^{k}\right\|^{2} + 4\epsilon CL^{2} \left\|\rho_{N}^{k-1}\right\|^{2} + \epsilon L^{2} \left\|\rho_{N}^{k-2}\right\|^{2} + \frac{\epsilon}{2}CL^{2} \left\|\rho_{N}^{k-N_{s}}\right\|^{2} + \frac{\epsilon C}{2} \left\|g^{k} - \tilde{g}^{k}\right\|^{2},$$

namely,

$$D_{\tau}^{\beta} \|\rho_{N}^{k}\|^{2} \leq \frac{2}{\epsilon} \|\rho_{N}^{k}\|^{2} + 8\epsilon CL^{2} \|\rho_{N}^{k-1}\|^{2} + 2\epsilon L^{2} \|\rho_{N}^{k-2}\|^{2} + \epsilon CL^{2} \|\rho_{N}^{k-N_{s}}\|^{2} + \epsilon C \|g^{k} - \tilde{g}^{k}\|^{2}.$$

By means of Lemma 0.11 and since $\epsilon > 0$, there exists a positive constant $\tau^* = \sqrt[\beta]{1/(2\Gamma(2-\beta)\frac{2}{\epsilon})}$, when $\tau < \tau^*$, we have

$$\left\|\rho_{N}^{k}\right\|^{2} \leq \frac{2\epsilon C t_{k}^{\beta}}{\Gamma(1+\beta)} E_{\beta}(2\mu t_{k}^{\beta}) \max_{1 \leq k \leq M} \left\|g^{k} - \tilde{g}^{k}\right\|^{2},$$

with $\mu = 2/\epsilon + 8C\epsilon L^2/(a_0 - a_1) + 2C\epsilon L^2/(a_1 - a_2) + C\epsilon L^2/(a_{N_s-1} - a_{N_s})$. By choosing $\epsilon \ge 4$, we simply know that $\tau^* \ge 1$ for all $0 < \beta < 1$. Thus the scheme is unconditionally stable.

1.4.2 Convergence analysis

In this subsection, we investigate the convergence of a fully discrete scheme (1.33) using error estimation.

Theorem 1.4. Let $\{\Phi^k\}_{k=-N_s}^M$ and $\{\Phi_N^k\}_{k=-N_s}^M$ be the exact and numerical solutions of equation (1.1) and the proposed scheme (1.33), respectively. Also, let $\Phi \in C^2([0,T]; L^2(\Omega)) \cap C^1([0,T]; H^s(\Omega))$. Then for a positive constant C independent of N and τ , the following statement is valid

$$|\Phi^k - \Phi^k_N|_{\alpha/2} \le C(N^{\alpha/2-s} + N^{-r} + \tau^{2-\beta}) , \ 1 \le k \le M,$$
 (1.36)

where the variable r denotes the regularity order of the source term.

Proof. Denote $\Phi^k - \Phi_N^k = e_N^k = (\Phi^k - \pi_N^{\frac{\alpha}{2},0} \Phi^k) + (\pi_N^{\frac{\alpha}{2},0} \Phi^k - \Phi_N^k) \stackrel{\Delta}{=} \tilde{e}_N^k + \hat{e}_N^k$. The weak formulation of equation (1.1) is

$$\begin{pmatrix} {}^{C}_{0}D^{\beta}_{t}\Phi^{k}, \upsilon_{N} \end{pmatrix} + A\left(\Phi^{k}, \upsilon_{N}\right) = \left(f\left(\Phi^{k}, \Phi^{k-N_{s}}\right), \upsilon_{N}\right) + \left(g^{k}, \upsilon_{N}\right).$$
(1.37)

Subtracting (1.33) from (1.37) and owing to the definition of orthogonal projection, the error equation satisfies

$$(D^{\beta}_{\tau}\hat{e}^{k}_{N}, \upsilon_{N}) + A(\hat{e}^{k}_{N}, \upsilon_{N}) \stackrel{\Delta}{=} \mathcal{E}^{k}_{1} + \mathcal{E}^{k}_{2} + \mathcal{E}^{k}_{3} + \mathcal{E}^{k}_{4}, \qquad (1.38)$$

where

$$\begin{aligned} \mathcal{E}_{1}^{k} &= \left(I_{N} f(\Phi^{k}, \Phi^{k-N_{s}}) - I_{N} f(2\Phi_{N}^{k-1} - \Phi_{N}^{k-2}, \Phi_{N}^{k-N_{s}}), \upsilon_{N} \right), \\ \mathcal{E}_{2}^{k} &= \left(f(\Phi^{k}, \Phi^{k-N_{s}}) - I_{N} f(\Phi^{k}, \Phi^{k-N_{s}}), \upsilon_{N} \right), \\ \mathcal{E}_{3}^{k} &= \left(D_{\tau}^{\beta} \pi_{N}^{\frac{\alpha}{2}, 0} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta} \Phi^{k}, \upsilon_{N} \right), \\ \mathcal{E}_{4}^{k} &= \left(g^{k} - I_{N} g^{k}, \upsilon_{N} \right). \end{aligned}$$

We next estimate the right-hand terms \mathcal{E}_1^k , \mathcal{E}_2^k , \mathcal{E}_3^k and \mathcal{E}_4^k . For the first term \mathcal{E}_1^k ,

$$\mathcal{E}_{1}^{k} = \left(I_{N}f\left(\Phi^{k}, \Phi^{k-N_{s}}\right) - I_{N}f\left(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}\right), \upsilon_{N}\right) \\
+ \left(I_{N}f\left(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}\right) - I_{N}f\left(2\Phi^{k-1}_{N} - \Phi^{k-2}_{N}, \Phi^{k-N_{s}}_{N}\right), \upsilon_{N}\right) \\
\stackrel{\Delta}{=} \mathcal{E}_{11}^{k} + \mathcal{E}_{12}^{k}.$$
(1.39)

Applying Taylor expansion holds

$$f\left(\Phi^{k}, \Phi^{k-N_{s}}\right) = f\left(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}\right) + \left(\Phi^{k} - 2\Phi^{k-1} + \Phi^{k-2}\right) f_{1}'\left(\xi, \Phi^{k-N_{s}}\right)$$
$$= f\left(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}\right) + \tilde{c}_{\Phi}\tau^{2},$$

furthermore, by means of Hölder inequality and Young's inequality, we have

$$\mathcal{E}_{11}^{k} \leq \left\| I_{N} f\left(\Phi^{k}, \Phi^{k-N_{s}}\right) - I_{N} f\left(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}\right) \right\| \|v_{N}\| \\ \leq C \left\| f\left(\Phi^{k}, \Phi^{k-N_{s}}\right) - f\left(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}\right) \right\| \|v_{N}\| \\ \leq \frac{\epsilon}{2} \tilde{c}_{\Phi} \tau^{4} + \frac{1}{2\epsilon} \|v_{N}\|^{2}.$$
(1.40)

Invoking the Lipschitz condition (1.32) and using Hölder inequality side by side to Young inequality, we deduce that

$$\mathcal{E}_{12}^{k} \leq LC \left(\left\| 2e_{N}^{k-1} - e_{N}^{k-2} \right\| + \left\| e_{N}^{k-N_{s}} \right\| \right) \left\| v_{N} \right\| \\
\leq LC \left(\left\| 2\hat{e}_{N}^{k-1} - \hat{e}_{N}^{k-2} \right\| + \left\| \hat{e}_{N}^{k-N_{s}} \right\| + \left\| 2\tilde{e}_{N}^{k-1} - \tilde{e}_{N}^{k-2} \right\| + \left\| \tilde{e}_{N}^{k-N_{s}} \right\| \right) \left\| v_{N} \right\| \\
\leq \frac{8\epsilon}{2}CL^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + \frac{2\epsilon}{2}CL^{2} \left\| \hat{e}_{N}^{k-2} \right\|^{2} + \frac{\epsilon}{2}L^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\|^{2} + \frac{8\epsilon}{2}CL^{2} \left\| \tilde{e}_{N}^{k-1} \right\|^{2} \\
+ \frac{2\epsilon}{2}CL^{2} \left\| \tilde{e}_{N}^{k-2} \right\|^{2} + \frac{\epsilon}{2}CL^{2} \left\| \tilde{e}_{N}^{k-N_{s}} \right\|^{2} + \frac{1}{2\epsilon} \left\| v_{N} \right\|^{2}.$$
(1.41)

Moreover, owing to Lemmas 0.2 and 0.3, it holds

$$\begin{aligned} \left\| \tilde{e}_{N}^{k-1} \right\|^{2} &\leq \frac{C}{C_{1}} N^{\alpha - 2s} \left\| \Phi^{k-1} \right\|_{s}^{2}; \\ \left\| \tilde{e}_{N}^{k-2} \right\|^{2} &\leq \frac{C}{C_{1}} N^{\alpha - 2s} \left\| \Phi^{k-2} \right\|_{s}^{2}; \\ \left\| \tilde{e}_{N}^{k-N_{s}} \right\|^{2} &\leq \frac{C}{C_{1}} N^{\alpha - 2s} \left\| \Phi^{k-N_{s}} \right\|_{s}^{2}. \end{aligned}$$
(1.42)

Then, (1.41) becomes

$$\mathcal{E}_{12}^{k} \leq 4\epsilon CL^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + \epsilon CL^{2} \left\| \hat{e}_{N}^{k-2} \right\|^{2} + \frac{\epsilon}{2} CL^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\|^{2} \\ + \frac{C}{C_{1}} N^{\alpha-2s} \left\| \Phi \right\|_{s}^{2} + \frac{1}{2\epsilon} \left\| v_{N} \right\|^{2}.$$
(1.43)

Substituting (1.40) and (1.43) into (1.39), we can derive that

$$\mathcal{E}_{1}^{k} \leq \frac{1}{\epsilon} \left\| v_{N} \right\|^{2} + 4\epsilon CL^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + \epsilon CL^{2} \left\| \hat{e}_{N}^{k-2} \right\|^{2} + \frac{\epsilon}{2} CL^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\|^{2} + \frac{C}{C_{1}} N^{\alpha-2s} \left\| \Phi \right\|_{s}^{2} + \frac{\epsilon}{2} \tilde{c}_{\Phi} \tau^{4}.$$
(1.44)

For the second term \mathcal{E}_2^k , by means of Hölder inequality, Young's inequality and Lemma 0.5, it holds

$$\mathcal{E}_{2}^{k} \leq \frac{\epsilon}{2} C N^{-2r} \|\Phi\|_{s}^{2} + \frac{1}{2\epsilon} \|\upsilon_{N}\|^{2}, \qquad (1.45)$$

For the third term \mathcal{E}_3^k , it holds

$$\begin{aligned} \mathcal{E}_{3}^{k} &= \left(D_{\tau}^{\beta} \pi_{N}^{\frac{\alpha}{2},0} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta} \pi_{N}^{\frac{\alpha}{2},0} \Phi^{k}, \upsilon_{N} \right) + \left({}_{0}^{C} D_{t}^{\beta} \pi_{N}^{\frac{\beta}{2},0} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta} \Phi^{k}, \upsilon_{N} \right) \\ &= \left(\pi_{N}^{\frac{\alpha}{2},0} \left(D_{\tau}^{\beta} \Phi^{k} - {}_{0}^{C} D_{t}^{\alpha} \Phi^{k} \right), \upsilon_{N} \right) - \left({}_{0}^{C} D_{t}^{\beta} \tilde{e}_{N}^{k}, \upsilon_{N} \right) \\ &= \stackrel{\Delta}{=} \mathcal{E}_{31}^{k} + \mathcal{E}_{32}^{k}, \end{aligned}$$
(1.46)

by combining the results of (1.3), the Hölder inequality, and the Young inequality, we obtain the following

$$\begin{aligned} \mathcal{E}_{31}^{k} &\leq \frac{\epsilon}{2} \left\| \pi_{N}^{\frac{\alpha}{2},0} \left(D_{\tau}^{\beta} u^{k} - {}_{0}^{C} D_{t}^{\beta} \Phi^{k} \right) \right\|^{2} + \frac{1}{2\epsilon} \| v_{N} \|^{2} \\ &\leq \frac{\epsilon}{2} C \left\| D_{\tau}^{\beta} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta} \Phi^{k} \right\|^{2} + \frac{1}{2\epsilon} \| v_{N} \|^{2} \\ &\leq \frac{\epsilon}{2} C_{1,\Phi} \tau^{4-2\beta} + \frac{1}{2\epsilon} \| v_{N} \|^{2}, \end{aligned}$$

furthermore, according to Lemma 0.2, we have

$$\mathcal{E}_{32}^{k} \leq \frac{\epsilon}{2} C N^{\alpha - 2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi^{k} \right\|_{s}^{2} + \frac{1}{2\epsilon} \left\| v_{N} \right\|^{2} \\ \leq \frac{\epsilon}{2} C N^{\alpha - 2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi \right\|_{s}^{2} + \frac{1}{2\epsilon} \left\| v_{N} \right\|^{2}.$$

Thus (1.46) becomes

$$\mathcal{E}_{3}^{k} \leq \frac{\epsilon}{2} C N^{\alpha-2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi \right\|_{s}^{2} + \frac{\epsilon}{2} C_{2,\Phi} \tau^{4-2\beta} + \frac{1}{\epsilon} \left\| \upsilon_{N} \right\|^{2}.$$

$$(1.47)$$

For the fourth term \mathcal{E}_4^k , it holds by invoking Remark 0.2

$$\mathcal{E}_{4}^{k} \leq \frac{\epsilon}{2} C N^{\alpha - 2r} \|\Phi\|_{r}^{2} + \frac{1}{2\epsilon} \|\upsilon_{N}\|^{2}.$$
(1.48)

Substituting (1.44), (1.45), (1.47) and (1.48) into (1.38), we can infer that

$$(D_{\tau}^{\beta} \hat{e}_{N}^{k}, \upsilon_{N}) + A(\hat{e}_{N}^{k}, \upsilon_{N})$$

$$\leq \frac{5}{2\epsilon} \|\upsilon_{N}\|^{2} + 4\epsilon CL^{2} \|\hat{e}_{N}^{k-1}\|^{2} + \epsilon CL^{2} \|\hat{e}_{N}^{k-2}\|^{2} + \frac{\epsilon}{2} CL^{2} \|\hat{e}_{N}^{k-N_{s}}\|^{2} + \tilde{\mathcal{R}},$$

$$(1.49)$$

where

$$\tilde{\mathcal{R}} = \epsilon \tilde{C} N^{\alpha - 2s} \left(\left\| {}_{0}^{C} D_{t}^{\beta} \Phi \right\|_{s}^{2} + \left\| \Phi \right\|_{s}^{2} \right) + \epsilon \tilde{C} N^{-2r} \left\| \Phi \right\|_{r}^{2} + \epsilon \tilde{C}_{\Phi} \tau^{4 - 2\beta}.$$

Taking $v_N = \hat{e}_N^k$ in (1.49) and applying Lemma 0.7, we can conclude that

$$\frac{1}{2}D_{\tau}^{\beta} \left\| \hat{e}_{N}^{k} \right\|^{2} + \left| \hat{e}_{N}^{k} \right|_{\alpha/2}^{2} \\ \leq \frac{5}{2\epsilon} \left\| \hat{e}_{N}^{k} \right\|^{2} + 4\epsilon CL^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + \epsilon CL^{2} \left\| \hat{e}_{N}^{k-2} \right\|^{2} + \frac{\epsilon}{2} CL^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\|^{2} + \tilde{\mathcal{R}},$$

namely,

$$D_{\tau}^{\beta} \left\| \hat{e}_{N}^{k} \right\|^{2} \leq \frac{5}{\epsilon} \left\| \hat{e}_{N}^{k} \right\|^{2} + 8\epsilon CL^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + 2\epsilon CL^{2} \left\| \hat{e}_{N}^{k-2} \right\|^{2} + \epsilon CL^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\|^{2} + \mathcal{R},$$

with $\mathcal{R} = 2\tilde{\mathcal{R}}$. By means of Lemma 0.11 and since $\epsilon > 0$, there exists a positive constant $\tau^* = \sqrt[\beta]{1/(2\Gamma(2-\beta)\frac{5}{\epsilon})}$, when $\tau < \tau^*$, we have

$$\left\| \hat{e}_{N}^{k} \right\|^{2} \leq \frac{2\mathcal{R}t_{k}^{\beta}}{\Gamma(1+\beta)} E_{\beta}(2\mu t_{k}^{\beta}),$$

with $\mu = 5/\epsilon + 8\epsilon CL^2/(a_0 - a_1) + 2C\epsilon L^2/(a_1 - a_2) + C\epsilon L^2/(a_{N_s-1} - a_{N_s})$. By choosing $\epsilon \ge 10$, we simply know that $\tau^* \ge 1$ for all $0 < \beta < 1$. Thus the scheme is unconditionally convergent. Finally, by means of triangle inequality and Lemma 0.2, we complete the proof of (1.36).

1.5 Numerical simulations

Some numerical experiments are performed here to clarify the convergence orders of the considered scheme in time and space. We also show the impact of time and space fractional orders on the behavior of the dynamics for the solution of nonlinear delay reaction-diffusion equations. To examine the temporal and spatial convergence orders separately, the orders of convergence in time and space shall be determined from the L^2 -error norms defined as:

Order =
$$\frac{\ln(\|e(N,M_1)\| / \|e(N,M_2)\|)}{\ln(M_1/M_2)}$$
, (1.50)

where $M_1 \neq M_2$.

Example 1.1. Consider the nonlinear delay reaction-diffusion problem

$$\frac{\partial^{\beta}\Phi}{\partial t^{\beta}}(x,t) = \frac{\partial^{\alpha}\Phi}{\partial |x|^{\alpha}}(x,t) - 2\Phi(x,t) + \frac{\Phi(x,t-0.1)}{1+\Phi^{2}(x,t-0.1)} + g(x,t), \ x \in (0,1), \ t \in (0,1],$$
(1.51)

where g(x,t) is a given function such that problem (1.51) has the exact solution $\frac{t^2}{\Gamma(3)}x^2(1-x)^2$.

In Table 1, we list the L^2 -errors and corresponding convergence orders with $\alpha - 1 = \beta = 0.1, 0.5, 0.9, N = 50$. We can see that these results confirm the expected theoretical order convergence in time. The convergence orders in space are depicted for different values of α and β at M = 500 in Figure 1.1. All the convergence results are in agreement with the theoretical results.

Table 1: The L^2 -errors and their convergence orders versus τ , α and β with N = 50 for example 1.1.

τ	$\alpha - 1 = \beta = 0.1$		$\alpha - 1 = \beta = 0.5$		$\alpha - 1 = \beta = 0.9$	
	Error	Order	Error	Order	Error	Order
0.1/5	2.612×10^{-7}		4.076×10^{-6}		2.449×10^{-5}	
0.1/10	7.466×10^{-8}	1.807	1.454×10^{-6}	1.487	1.143×10^{-5}	1.099
0.1/15	3.588×10^{-8}	1.807	7.943×10^{-7}	1.491	7.319×10^{-6}	1.100
0.1/20	2.156×10^{-8}	1.771	5.168×10^{-7}	1.494	5.334×10^{-6}	1.100
0.1/25	1.481×10^{-8}	1.682	3.702×10^{-7}	1.495	4.173×10^{-6}	1.100

Example 1.2. We consider the nonlinear delay reaction-diffusion equation 1.51 with the non-smooth exact solution $(t+1)^{\beta}x^2(1-x)^2$. We apply the proposed scheme to solve Example 1.2 and also choose N = 50, the temporal convergence rates are given in Table 2. The time accuracy is not tending to the expected temporal convergence order $2 - \beta$ and can go to β order. This can be understood due to the singularity of the solution with respect to time which clears the drawback of handling the smooth L1 formula in our approximation scheme (1.8). This will motivate us to try to construct a nonsmooth L1 scheme that can capture perfectly the



Figure 1.1 – Convergence order in space direction for different values of α and β at $\tau = 0.1/50$.

time derivative discontinuities behavior of the solutions of the equations at multiple points generated by the time delay and the Caputo fractional derivative. Moreover, the spectral accuracy of L^2 -error is given in Table 2 with different values N which also demonstrates the theoretical analysis.

example 1.2.							
au	N = 50		N	$\tau = 1/500$			
	Error	Order		Error	Order		
0.1/5	6.690×10^{-7}		5	2.835×10^{-4}	$N^{-5.075}$		
0.1/10	2.458×10^{-7}	1.444	10	2.714×10^{-5}	$N^{-4.566}$		
0.1/15	1.394×10^{-7}	1.398	15	2.140×10^{-6}	$N^{-4.820}$		
0.1/20	9.568×10^{-8}	1.309	20	1.738×10^{-6}	$N^{-4.427}$		
0.1/25	7.353×10^{-8}	1.180	25	2.337×10^{-7}	$N^{-4.743}$		

Table 2: The L^2 -errors and their convergence orders with $\alpha - 1 = \beta = 0.5$ for example 1.2.

Chapter 2 Numerical method for the generalized nonlinear multi-term time-space fractional reaction-diffusion equations with delay

In this chapter, we develop and analyze a linearized finite difference/Galerkin-Legendre spectral scheme for the generalized nonlinear multiterm Caputo-time fractional-order reaction-diffusion equation with time delay and Riesz-space fractional derivatives. The temporal fractional orders in the considered model are taken as $(0 < \beta_0 < \beta_1 < \beta_2 < \cdots < \beta_m < 1)$. The problem is first approximated by the L1 difference method on the temporal direction, and then the Galerkin-Legendre spectral method is applied to the spatial discretization. Armed by an appropriate form of discrete fractional Grönwall inequalities, the stability, and convergence of the fully discrete scheme are investigated by discrete energy estimates. We show that the proposed method is stable and has a convergent order of $2 - \beta_m$, in time, and an exponential rate of convergence in space. We finally provide some numerical experiments to show the efficacy of the theoretical results.

2.1 Preliminary results and problem formulation

Multi-term time-fractional differential equations have gained significant attention in recent years. The ability of these equations to represent complicated multi-rate physical processes is a driving factor in their development (see, e.g., [137– 139]). The motivation for proposing such equations was to improve the modeling accuracy by accurately depicting the anomalous diffusion process [140], accurately modeling various types of viscoelastic damping [141], and accurately reproducing the unsteady flow of a fractional Maxwell fluid [142] and Oldroyd-B fluid [143]. The literature has paid considerable attention to multi-term fractional partial differential equations. However, a few works investigated cases with a two-term time-fractional differential equation that contains specific instances of the fractional diffusion-wave problem (see, for example, [144; 145]). Daftardar and Bhalekar [146] considered the multi-term time-fractional diffusion wave equation with constant coefficients. Through the use of a domain decomposition technique, they were able to derive the linear and nonlinear diffusion-wave equations of fractional order. Luchko [147] used an appropriate maximum principle and the Fourier technique to study the existence, uniqueness, and a priori estimates for the multi-term time-fractional diffusion equation with variable coefficients. A new analytic technique for solving three types of multi-term time-space fractional advection-diffusion equations with non-homogeneous Dirichlet boundary conditions was proposed in [148], based on Luchko's theorem and the equivalent relationship between the Laplacian operator and the Riesz fractional derivative. Ding and Jiang [149] used the technique of spectral representation of the fractional Laplacian operator in order to provide the analytical solutions for the multi-term time-space fractional advection-diffusion equations with mixed boundary conditions. For the solution of initial-boundary value problems of multi-term time-fractional diffusion equations, Li and his coauthors [150] examined the well-posedness and long-time asymptotic behavior of the equations. To solve the multi-term time-fractional diffusion equations, Zaky introduced a very useful method in [151], which was referred to as the Legendre spectral tau algorithm. Hendy [152] presented a numerical treatment for solving a class of one-dimensional multi-term time-space fractional advection-diffusion equations with a temporal delay of the functional type. Hendy and De Staelen [153] developed a high-order numerical approximation approach for multi-term time convection diffusion wave equations with a non-linear fixed time delay. To solve a coupled system of nonlinear multi--term time-space fractional diffusion equations over a nonuniform temporal mesh, Hendy and Zaky [154] developed an effective finite difference/spectral approach. Very recently, Zaky et al. [86] presented a discrete fractional Grönwall inequality that is consistent with the analysis of multi-term time-fractional partial differential equations. The key advantage of the proposed discrete Grönwall inequality over earlier efforts was that it can be utilized to provide an optimal error estimates for multi-term fractional problems with nonlinear delay. Inspired by these inequalities, we can state and prove the convergence and stability estimates for our proposed fully-discrete scheme.

Single-term fractional differential equations are often unable to describe some of the changing characteristics of the systems accurately. However, several multi-term fractional differential equations provide us with new tools to solve such problems. The multi-term time-fractional diffusion equation is useful not only for modeling the behavior of viscoelastic fluids and rheological materials [155] but also for approximating distributed-order differential equations [71]. Hence, studies on multi-term time-fractional differential equations have become important and useful for different applications. The multi-term time-fractional diffusion equation, whose weight function is taken into the linear combination of the Dirac δ -functions, is an important special case of the time-fractional diffusion equation of distributed order [156]. In this chapter, we consider the numerical approximations of the following generalized nonlinear multi-term time-space fractional reaction-diffusion equations with delay

$$\sum_{r=0}^{m} q_r \frac{\partial^{\beta_r} \Phi}{\partial t^{\beta_r}} = \kappa \frac{\partial^{\alpha} \Phi}{\partial |x|^{\alpha}} + f\left(\Phi(x,t), \Phi(x,t-s)\right) + g(x,t), \quad x \in \Omega, \quad t \in I, \quad (2.1)$$

endowed with initial-boundary conditions of the form

$$\begin{cases} \Phi(x,t) = \psi(x,t), & x \in \Omega, \quad t \in [-s,0], \\ \Phi(a,t) = \Phi(b,t) = 0, \quad t \in I, \end{cases}$$
(2.2)

where $\Omega = (a, b) \subset \mathbb{R}$ and $I = (0,T] \subset \mathbb{R}$ are space and time domains, respectively. And $(0 < \beta_0 < \beta_1 < \beta_2 < \cdots < \beta_m < 1)$ is the time fractional order such that the time-fractional derivative is understood in the sense of Caputo, whereas $1 < \alpha < 2$, is the space fractional order. The positive constants κ , and s, denote the diffusion, temporal delay parameters, respectively. The parameters q_r are positive.

2.2 Derivation of Numerical Scheme

Here, we provide a fully discrete scheme for the problem (2.1)-(2.2) based on the L1-type approximation for the Caputo time-fractional derivative and the Legendre-Galerkin spectral method in space. We first discuss the temporal discretization of the proposed method and then go into detail about spatial discretization.

2.2.1 Temporal discretization

We choose a time step given by $\tau = \frac{s}{N_s}$, where N_s is a positive integer, in order to uniformly discretize the temporal domain I. This defines a class of uniform partitions denote by $t_n = n\tau$, for each $-N_s \leq n \leq M$, where $M = \lceil \frac{T}{\tau} \rceil$. Denote $\Phi^n = \Phi(., t_n)$, then the following expressions can be used to get the L1 estimate for the Caputo-time fractional derivative (6) of order $0 < \beta_r < 1, r = 0, 1, 2, ..., m$ at the time t_n , as

$$\begin{split} \sum_{r=0}^{m} q_{r} \frac{\partial^{\beta_{r}} \Phi}{\partial t^{\beta_{r}}} \bigg|_{t=t_{n}} &= \sum_{r=0}^{m} q_{r} \int_{0}^{t_{n}} \Phi'(x,\eta) \omega_{1-\beta_{r}}(t_{n}-\eta) d\eta \\ &= \sum_{r=0}^{m} \frac{q_{r}}{\Gamma(1-\beta_{r})} \sum_{i=1}^{n} \frac{\Phi(x,t_{i}) - \Phi(x,t_{i-1})}{\tau} \int_{t_{i-1}}^{t_{i}} (t_{n}-\eta)^{-\beta_{r}} d\eta + r_{\tau}^{n} \\ &= \sum_{r=0}^{m} \frac{q_{r}}{\Gamma(2-\beta_{r})\tau^{\beta_{r}}} \sum_{i=1}^{n} a_{n-i}^{\beta_{r}} \left(\Phi(x,t_{i}) - \Phi(x,t_{i-1})\right) + r_{\tau}^{n}, \end{split}$$
(2.3)

where the kernel $\omega_{\beta_r}(t) = \frac{t^{\beta_r-1}}{\Gamma(\beta_r)}$, t > 0, and $a_j^{\beta_r} = (j+1)^{1-\beta_r} - j^{1-\beta_r}$, for each $j \ge 0$. If $\Phi \in C^2([0,T]; L^2(\Omega))$ then there exists a constant C > 0 such that the truncation error r_{τ}^n satisfies $||r_{\tau}^n|| \le C\tau^{2-\beta_m}$, for each $n = 0, 1, \ldots, M$ (see [68]). This allows us to give the following definition for the multi-term discrete time-fractional difference operator.

Definition 2.1. Let $\{\Phi^n\}_{n=0}^M$ a sequence of real functions defined on Ω . We define the multi-term discrete time-fractional difference operator $\sum_{r=0}^m q_r D_{\tau}^{\beta_r}$ by

$$\sum_{r=0}^{m} q_r D_{\tau}^{\beta_r} \Phi^n = \sum_{r=0}^{m} \frac{q_r}{\Gamma(2-\beta_r)\tau^{\beta_r}} \sum_{i=1}^{n} a_{n-i}^{\beta_r} \delta_t \Phi^i = \sum_{r=0}^{m} \frac{q_r}{\Gamma(2-\beta_r)\tau^{\beta_r}} \sum_{i=0}^{n} b_{n-i}^{\beta_r} \Phi^i,$$
(2.4)

for all values of n = 1, ..., M. In this expression, $\delta_t \Phi^i = \Phi^i - \Phi^{i-1}$, and the constants are defined by $b_0^{\beta_r} = a_0^{\beta_r}$, $b_n^{\beta_r} = -a_{n-1}^{\beta_r}$, $b_{n-i}^{\beta_r} = a_{n-i}^{\beta_r} - a_{n-i-1}^{\beta_r}$, for each i = 1, ..., n-1.

In order to provide a semi-discretized form of (2.1) at each time t_n , we approximate the time-fractional term through (2.4). In addition, Taylor approximations

are used to approximate the nonlinear source function in a linear style. As a consequence, we obtain the discrete-time system

$$\begin{cases} \sum_{r=0}^{m} q_r D_{\tau}^{\beta_r} \Phi^n = \frac{\partial^{\alpha} \Phi^n}{\partial |x|^{\alpha}} + f(2\Phi^{n-1} - \Phi^{n-2}, \Phi^{n-N_s}) + g^n(x), \ 1 \le n \le M, \ \forall x \in \Omega, \\ \Phi^n(x) = \psi(x), \quad -N_s \le n \le 0, \quad x \in \Omega. \end{cases}$$

$$(2.5)$$

Let us introduce the parameter $\lambda_r := \frac{q_r}{\Gamma(2-\beta_r)\tau^{\beta_r}}$. Then the semi-scheme (2.5) can be rewritten in the following equivalent form given below:

$$\sum_{r=0}^{m} \lambda_r a_0^{\beta_r} \Phi^n - \kappa \frac{\partial^{\alpha} \Phi^n}{\partial |x|^{\alpha}} = \sum_{r=0}^{m} \lambda_r \ a_{n-1}^{\beta_r} \Phi^0 - \sum_{r=0}^{m} \lambda_r \sum_{i=1}^{n-1} b_{n-i}^{\beta_r} \Phi^i + f(2\Phi^{n-1} - \Phi^{n-2}, \Phi^{n-N_s}) + g^n(x), \quad \forall n = 1, \dots, M.$$
(2.6)

2.2.2 Spatial discretization

We define the following function space to give an appropriate base functions such that the boundary conditions are satisfied exactly as clarified in spectral methods for space-fractional differential equations [118; 133]

$$\mathcal{W}_{N}^{0} = \text{span} \{ \varphi_{n}(x) : n = 0, 1, \dots, N - 2 \},$$
 (2.7)

where, for each $\hat{x} \in [-1, 1]$, the function φ_n is given by

$$\varphi_n(x) = L_n(\hat{x}) - L_{n+2}(\hat{x}) = \frac{2n+3}{2(n+1)}(1-\hat{x}^2)J_n^{1,1}(\hat{x}),$$

and $x = \frac{1}{2}((b-a)\hat{x} + a + b) \in [a, b]$. Thus, the fully discrete *L*1-Galerkin spectral scheme consists of the set of approximations $\Phi_N^n \in \mathcal{W}_N^0$, satisfying the following system:

$$\begin{cases} \sum_{r=0}^{m} \lambda_r a_0^{\beta_r} \left(\Phi_N^n, \upsilon\right) - \kappa \left(\frac{\partial^{\alpha} \Phi_N^n}{\partial \left|x\right|^{\alpha}}, \upsilon\right) = \sum_{r=0}^{m} \lambda_r a_{n-1}^{\beta_r} \left(\Phi_N^0, \upsilon\right) - \sum_{r=0}^{m} \lambda_r \sum_{i=1}^{n-1} b_{n-i}^{\beta_r} \left(\Phi_N^i, \upsilon\right) + \left(I_N f \left(2\Phi_N^{n-1} - \Phi_N^{n-2}, \Phi_N^{n-N_s}\right), \upsilon\right) + \left(I_N g^n(x), \upsilon\right), \ \forall \upsilon \in \mathcal{W}_N^0, \ \forall n = 1, \dots, M, \\ \Phi_N^n = \pi_N^{1,0} \psi(t_n, x), \quad -N_s \le n \le 0, \end{cases}$$

$$(2.8)$$

where $\pi_N^{1,0}$ is an appropriate projection operator. Next, we expand the approximate solution as

$$\Phi_N^n = \sum_{i=0}^{N-2} \hat{\Phi}_i^n \varphi_i(x), \qquad (2.9)$$

where $\hat{\Phi}_i^n$ are the unknown expansion coefficients to be specified. Substituting this expression into (2.8) and letting $v = \varphi_k$, for each $0 \le k \le N - 2$, we obtain the following matrix representation of the uniform L_1 -Galerkin spectral scheme

$$\left(\sum_{r=0}^{m} \lambda_r a_0^{\beta_r} \bar{M} - \kappa c_\alpha (S + S^T)\right) U^n = K^{n-1} + H^{n-1} + G^n.$$
(2.10)

The notations in this expression are given by the system of identities

$$\begin{cases} s_{ij} = \int_{\Omega} {}_{a} D_{x}^{\frac{\alpha}{2}} \varphi_{i}(x)_{x} D_{b}^{\frac{\alpha}{2}} \varphi_{j}(x) dx, & S = (s_{ij})_{i,j=0}^{N-2}, \\ m_{ij} = \int_{\Omega} \varphi_{i}(x) \varphi_{j}(x) dx, & \bar{M} = (m_{ij})_{i,j=0}^{N-2}, \\ h_{i}^{n-1} = \int_{\Omega} \varphi_{i}(x) I_{N} f(2\Phi_{N}^{n-1} - \Phi_{N}^{n-2}, \Phi_{N}^{n-N_{s}}) dx, & H^{n-1} = (h_{0}^{n-1}, h_{1}^{n-1}, \dots, h_{N-2}^{n-1})^{\top}, \\ g_{i}^{n} = \int_{\Omega} \varphi_{i}(x) I_{N} g^{n} dx, & G^{n} = (g_{0}^{n}, g_{1}^{n}, \dots, g_{N-2}^{n})^{\top}, \\ U^{n} = (\hat{\Phi}_{0}^{n}, \hat{\Phi}_{1}^{n}, \dots, \hat{\Phi}_{N-2}^{n})^{\top}, & K^{n-1} = -\sum_{r=0}^{m} \lambda_{r} \sum_{j=0}^{n-1} b_{n-j}^{\beta_{r}} \bar{M} U^{j}. \end{cases}$$

The elements of the stiffness matrix S and the mass matrix \overline{M} can be easily calculated using lemma 1.1.

2.3 Theoretical analysis

The purpose of this section is to study the efficiency of the fully discrete Galerkin spectral methods for the (2.1)-(2.2). We start with stability analysis and give the theorem of stability in the first subsection. The second subsection is devoted to the convergence analysis and the theorem of convergence is given there. For the theoretical analysis requirements, we assume that the function f satisfies the following Lipschitz condition

$$|f(\Phi_1, v_1) - f(\Phi_2, v_2)| \le L \left(|\Phi_1 - \Phi_2| + |v_1 - v_2| \right), \qquad (2.11)$$

where L is a positive constant.

2.3.1 Stability analysis

The weak formulation of a fully discrete scheme is as follows: find $\{\Phi_N^k\}_{k=1}^M \in \mathcal{P}_N$, such that satisfying the following

$$\left(\sum_{r=0}^{m} q_r D_{\tau}^{\beta_r} \Phi_N^k, \upsilon_N\right) + A\left(\Phi_N^k, \upsilon_N\right)$$
$$= \left(I_N f(2\Phi_N^{k-1} - \Phi_N^{k-2}, \Phi_N^{k-N_s}), \upsilon_N\right) + \left(I_N g^k, \upsilon_N\right), \quad \forall \upsilon_N \in \mathcal{P}_N, \quad (2.12)$$

with

$$\Phi_N^k = \pi_N^{1,0} \varphi^k, \ -N_s \le k \le 0.$$

It is a linear iterative scheme which means that we need only to get a solution to a system of linear equations at each time level. The well-posedness of the proposed scheme, that is, its unique solvability and continuous dependency on the initial-boundary conditions, is sufficient to validate the hypotheses of the well-known Lax– Milgram's lemma [136]. More specifically, in terms of (2.12), we see that the bilinear form $A(\cdot, \cdot)$ is continuous and coercive in $H_0^{\alpha/2} \times H_0^{\alpha/2}$. Assume that $\{\tilde{\Phi}_N^k\}_{k=1}^M$ is the solution of the variation form

$$\left(\sum_{r=0}^{m} q_r D_{\tau}^{\beta_r} \tilde{\Phi}_N^k, \upsilon_N\right) + A\left(\tilde{\Phi}_N^k, \upsilon_N\right) \\
= \left(I_N f(2\tilde{\Phi}_N^{k-1} - \tilde{\Phi}_N^{k-2}, \tilde{\Phi}_N^{k-N_s}), \upsilon_N\right) + \left(I_N \tilde{g}^k, \upsilon_N\right), \quad \forall \upsilon_N \in \mathcal{P}_N, \quad (2.13)$$

with initial conditions

$$\tilde{\Phi}_N^k = \pi_N^{1,0} \varphi^k, \quad -N_{\tilde{s}} \le k \le 0.$$

Now, we are ready to present the theorem of stability in the following context.

Theorem 2.1. The fully discrete scheme (2.12) is unconditionally stable in the sense that for all $\tau > 0$, it holds

$$\left\|\Phi_{N}^{k}-\tilde{\Phi}_{N}^{k}\right\|^{2} \leq C \max_{1\leq k\leq M}\left\|g^{k}-\tilde{g}^{k}\right\|^{2},$$

where C is a positive constant independent of N and τ . Proof. Denote $\rho_N^k = \Phi_N^k - \tilde{\Phi}_N^k$. Subtracting (2.13) from (2.12), it holds

$$\left(\sum_{r=0}^{m} q_r D_{\tau}^{\beta_r} \rho_N^k, \upsilon_N\right) + A\left(\rho_N^k, \upsilon_N\right)
= \left(I_N f\left(2\Phi_N^{k-1} - \Phi_N^{k-2}, \Phi_N^{k-N_{\tilde{s}}}\right) - I_N f\left(2\tilde{\Phi}_N^{k-1} - \tilde{\Phi}_N^{k-2}, \tilde{\Phi}_N^{k-N_s}\right), \upsilon_N\right)
+ \left(I_N g^k - I_N \tilde{g}^k, \upsilon_N\right).$$
(2.14)

According to (2.11) and using Hölder inequality and Young's inequality, we derive that for the first term

$$\begin{split} &\left(I_{N} f(2\Phi_{N}^{k-1} - \Phi_{N}^{k-2}, \Phi_{N}^{k-N_{s}}) - I_{N} f(2\tilde{\Phi}_{N}^{k-1} - \tilde{\Phi}_{N}^{k-2}, \tilde{\Phi}_{N}^{k-N_{s}}), \upsilon_{N}\right) \\ &\leq C L \left(\left\|2\rho_{N}^{k-1} - \rho_{N}^{k-2}\right\| + \left\|\rho_{N}^{k-N_{\tilde{s}}}\right\|\right) \|\upsilon_{N}\| \\ &\leq \frac{\epsilon}{2} C L^{2} \left\|2\rho_{N}^{k-1} - \rho_{N}^{k-2}\right\|^{2} + \frac{\epsilon}{2} C L^{2} \left\|\rho_{N}^{k-N_{\tilde{s}}}\right\|^{2} + \frac{1}{2\epsilon} \left\|\upsilon_{N}\right\|^{2} \\ &\leq 4\epsilon C L^{2} \left\|\rho_{N}^{k-1}\right\|^{2} + \epsilon L^{2} \left\|\rho_{N}^{k-2}\right\|^{2} + \frac{\epsilon}{2} C L^{2} \left\|\rho_{N}^{k-N_{\tilde{s}}}\right\|^{2} + \frac{1}{2\epsilon} \left\|\upsilon_{N}\right\|^{2}, \end{split}$$

and for the second term

$$\left(I_N g^k - I_N \tilde{g}^k, \upsilon_N\right) \leq \frac{\epsilon}{2} C \left\|g^k - \tilde{g}^k\right\|^2 + \frac{1}{2\epsilon} \left\|\upsilon_N\right\|^2.$$

Then (2.14) becomes

$$\left(\sum_{r=0}^{m} q_r D_{\tau}^{\beta_r} \rho_N^k, \upsilon_N \right) + A(\rho_N^k, \upsilon_N)$$

$$\leq \frac{1}{\epsilon} \|\upsilon_N\|^2 + 4\epsilon C L^2 \|\rho_N^{k-1}\|^2 + \epsilon L^2 \|\rho_N^{k-2}\|^2 + \frac{\epsilon}{2} C L^2 \|\rho_N^{k-N_{\tilde{s}}}\|^2 + \frac{\epsilon C}{2} \|g^k - \tilde{g}^k\|^2.$$

Taking $v_N = \rho_N^k$ and using (22) and (16), we can deduce that

$$\begin{split} &\sum_{r=0}^{m} \frac{q_{r}}{2} D_{\tau}^{\beta_{r}} \left\| \rho_{N}^{k} \right\|^{2} + \left| \rho \right|_{\alpha/2}^{2} \\ &\leq \frac{1}{\epsilon} \left\| \rho_{N}^{k} \right\|^{2} + 4\epsilon CL^{2} \left\| \rho_{N}^{k-1} \right\|^{2} + \epsilon L^{2} \left\| \rho_{N}^{k-2} \right\|^{2} + \frac{\epsilon}{2} CL^{2} \left\| \rho_{N}^{k-N_{\tilde{s}}} \right\|^{2} + \frac{\epsilon C}{2} \left\| g^{k} - \tilde{g}^{k} \right\|^{2}, \end{split}$$

namely,

$$\sum_{r=0}^{m} q_{r} D_{\tau}^{\beta_{r}} \left\| \rho_{N}^{k} \right\|^{2} \\ \leq \frac{2}{\epsilon} \left\| \rho_{N}^{k} \right\|^{2} + 8\epsilon C L^{2} \left\| \rho_{N}^{k-1} \right\|^{2} + 2\epsilon L^{2} \left\| \rho_{N}^{k-2} \right\|^{2} + \epsilon C L^{2} \left\| \rho_{N}^{k-N_{\tilde{s}}} \right\|^{2} + \epsilon C \left\| g^{k} - \tilde{g}^{k} \right\|^{2}.$$

By means of Lemma 0.12 and since $\epsilon > 0$, there exists a positive constant $\tau^* = \sqrt[\beta_m]{q_m/\left(2\Gamma(2-\beta_m)\frac{2}{\epsilon}\right)}$, when $\tau < \tau^*$, we have

$$\left\|\rho_N^k\right\|^2 \le \frac{2\epsilon C t_k^{\beta_m}}{q_m \Gamma(1+\beta_m)} E_{\beta_m} \left(2\mu t_k^{\beta_m}/q_m\right) \sum_{k=1}^M \left\|g^k - \tilde{g}^k\right\|^2,$$

with $\mu = 2/\epsilon + 8C\epsilon L^2/(a_0^{\beta_m} - a_1^{\beta_m}) + 2C\epsilon L^2/(a_1^{\beta_m} - a_2^{\beta_m}) + C\epsilon L^2/(a_{N_s-1}^{\beta_m} - a_{N_s}^{\beta_m}).$ Thus the scheme is unconditionally stable.

2.3.2 Convergence analysis

In this subsection, we investigate the convergence of the fully discrete scheme (2.12) using error estimation.

Theorem 2.2. Let $\{\Phi^k\}_{k=-N_s}^M$ and $\{\Phi_N^k\}_{k=-N_s}^M$ be the exact and numerical solutions of equation (2.1) and the proposed scheme (2.12), respectively. Also, let $\Phi \in C^2([0,T]; L^2(\Omega)) \cap C^1([0,T]; H^s(\Omega))$. Then for a positive constant C independent of N and τ , the following statement is valid

$$|\Phi^k - \Phi^k_N|_{\alpha/2} \le C(N^{\alpha/2-s} + N^{-r} + \tau^{2-\beta_m}) , \ 1 \le k \le M.$$
 (2.15)

Proof. Denote $\Phi^k - \Phi^k_N = e^k_N = (\Phi^k - \pi^{\frac{\alpha}{2},0}_N \Phi^k) + (\pi^{\frac{\alpha}{2},0}_N \Phi^k - \Phi^k_N) \stackrel{\Delta}{=} \tilde{e}^k_N + \hat{e}^k_N$. The weak formulation of equation (2.1) is

$$\left(\sum_{r=0}^{m} q_r \, {}_{0}^{C} D_t^{\beta_r} \Phi^k, \, \upsilon_N\right) + A\left(\Phi^k, \, \upsilon_N\right) = \left(f\left(\Phi^k, \Phi^{k-N_s}\right), \upsilon_N\right) + \left(g^k, \, \upsilon_N\right). \quad (2.16)$$

Subtracting (2.12) from (2.16) and owing to the definition of orthogonal projection, the error equation satisfies

$$\left(\sum_{r=0}^{m} q_r D_{\tau}^{\beta_r} \hat{e}_N^k, \upsilon_N\right) + A\left(\hat{e}_N^k, \upsilon_N\right) \stackrel{\Delta}{=} \mathcal{E}_1^k + \mathcal{E}_2^k + \mathcal{E}_3^k + \mathcal{E}_4^k, \qquad (2.17)$$

where

$$\begin{aligned} \mathcal{E}_{1}^{k} &= \left(I_{N} f(\Phi^{k}, \Phi^{k-N_{s}}) - I_{N} f(2\Phi_{N}^{k-1} - \Phi_{N}^{k-2}, \Phi_{N}^{k-N_{s}}), \upsilon_{N} \right), \\ \mathcal{E}_{2}^{k} &= \left(f(\Phi^{k}, \Phi^{k-N_{s}}) - I_{N} f(\Phi^{k}, \Phi^{k-N_{s}}), \upsilon_{N} \right), \\ \mathcal{E}_{3}^{k} &= \left(\sum_{r=0}^{m} q_{r} \left(D_{\tau}^{\beta_{r}} \pi_{N}^{\frac{\alpha}{2}, 0} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta_{r}} \Phi^{k} \right), \upsilon_{N} \right), \\ \mathcal{E}_{4}^{k} &= \left(g^{k} - I_{N} g^{k}, \upsilon_{N} \right). \end{aligned}$$

We next estimate the right-hand terms \mathcal{E}_1^k , \mathcal{E}_2^k , \mathcal{E}_3^k and \mathcal{E}_4^k . For the first term \mathcal{E}_1^k ,

$$\mathcal{E}_{1}^{k} = \left(I_{N}f\left(\Phi^{k}, \Phi^{k-N_{s}}\right) - I_{N}f(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}), \upsilon_{N}\right) + \left(I_{N}f(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}) - I_{N}f(2\Phi^{k-1}_{N} - \Phi^{k-2}_{N}, \Phi^{k-N_{s}}_{N}), \upsilon_{N}\right) \stackrel{\Delta}{=} \mathcal{E}_{11}^{k} + \mathcal{E}_{12}^{k}.$$
(2.18)

Applying Taylor expansion, it holds

$$f(\Phi^k, \Phi^{k-N_s}) = f(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_s}) + (\Phi^k - 2\Phi^{k-1} + \Phi^{k-2}) f_1'(\xi, \Phi^{k-N_s})$$
$$= f(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_s}) + \tilde{c}_{\Phi}\tau^2,$$

furthermore, by means of Hölder inequality and Young's inequality, we have

$$\mathcal{E}_{11}^{k} \leq \left\| I_{N} f(\Phi^{k}, \Phi^{k-N_{s}}) - I_{N} f(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}) \right\| \|\upsilon_{N}\| \\
\leq C \left\| f(\Phi^{k}, \Phi^{k-N_{s}}) - f(2\Phi^{k-1} - \Phi^{k-2}, \Phi^{k-N_{s}}) \right\| \|\upsilon_{N}\| \\
\leq \frac{\epsilon}{2} \tilde{c}_{\Phi} \tau^{4} + \frac{1}{2\epsilon} \|\upsilon_{N}\|^{2}.$$
(2.19)

According to (2.11) and using Hölder inequality side by side to Young inequality, we deduce that

$$\mathcal{E}_{12} \leq LC \left(\left\| 2e_N^{k-1} - e_N^{k-2} \right\| + \left\| e_N^{k-N_s} \right\| \right) \|v_N\| \\
\leq LC \left(\left\| 2\hat{e}_N^{k-1} - \hat{e}_N^{k-2} \right\| + \left\| \hat{e}_N^{k-N_s} \right\| + \left\| 2\tilde{e}_N^{k-1} - \tilde{e}_N^{k-2} \right\| + \left\| \tilde{e}_N^{k-N_s} \right\| \right) \|v_N\| \\
\leq \frac{8\epsilon}{2}CL^2 \left\| \hat{e}_N^{k-1} \right\|^2 + \frac{2\epsilon}{2}CL^2 \left\| \hat{e}_N^{k-2} \right\|^2 + \frac{\epsilon}{2}L^2 \left\| \hat{e}_N^{k-N_s} \right\|^2 + \frac{8\epsilon}{2}CL^2 \left\| \tilde{e}_N^{k-1} \right\|^2 \\
+ \frac{2\epsilon}{2}CL^2 \left\| \tilde{e}_N^{k-2} \right\|^2 + \frac{\epsilon}{2}CL^2 \left\| \tilde{e}_N^{k-N_s} \right\|^2 + \frac{1}{2\epsilon} \left\| v_N \right\|^2.$$
(2.20)

Moreover, owing to Lemmas 0.2 and 0.3, it holds

$$\begin{aligned} \left\| \tilde{e}_{N}^{k-1} \right\|^{2} &\leq \frac{C}{C_{1}} N^{\alpha-2s} \left\| \Phi^{k-1} \right\|_{s}^{2}, \\ \left\| \tilde{e}_{N}^{k-2} \right\|^{2} &\leq \frac{C}{C_{1}} N^{\alpha-2s} \left\| \Phi^{k-2} \right\|_{s}^{2}, \\ \left\| \tilde{e}_{N}^{k-N_{s}} \right\|^{2} &\leq \frac{C}{C_{1}} N^{\alpha-2s} \left\| \Phi^{k-N_{s}} \right\|_{s}^{2}. \end{aligned}$$

$$(2.21)$$

Then, (2.20) becomes

$$\mathcal{E}_{12}^{k} \leq 4\epsilon CL^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + \epsilon CL^{2} \left\| \hat{e}_{N}^{k-2} \right\|^{2} + \frac{\epsilon}{2} CL^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\|^{2} + \frac{C}{C_{1}} N^{\alpha-2s} \left\| \Phi \right\|_{s}^{2} + \frac{1}{2\epsilon} \left\| v_{N} \right\|^{2}.$$

$$(2.22)$$

Substituting (2.19) and (2.22) into (2.18), we can derive that

$$\mathcal{E}_{1}^{k} \leq \frac{1}{\epsilon} \|v_{N}\|^{2} + 4\epsilon CL^{2} \|\hat{e}_{N}^{k-1}\|^{2} + \epsilon CL^{2} \|\hat{e}_{N}^{k-2}\|^{2} + \frac{\epsilon}{2} CL^{2} \|\hat{e}_{N}^{k-N_{s}}\|^{2} + \frac{C}{C_{1}} N^{\alpha-2s} \|\Phi\|_{s}^{2} + \frac{\epsilon}{2} \tilde{c}_{\Phi} \tau^{4}.$$
(2.23)

For the second term \mathcal{E}_2^k , by means of Hölder inequality, Young's inequality and Lemma 0.5, it holds

$$\mathcal{E}_{2}^{k} \leq \frac{\epsilon}{2} C N^{-2r} \|\Phi\|_{s}^{2} + \frac{1}{2\epsilon} \|\upsilon_{N}\|^{2}.$$
(2.24)

For the third term \mathcal{E}_3^k , it holds

$$\mathcal{E}_{3}^{k} = \left(\sum_{r=0}^{m} q_{r} \left(D_{\tau}^{\beta_{r}} \pi_{N}^{\frac{\alpha}{2},0} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta_{r}} \pi_{N}^{\frac{\alpha}{2},0} \Phi^{k}\right), \upsilon_{N}\right) \\
+ \left(\sum_{r=0}^{m} q_{r} \left({}_{0}^{C} D_{t}^{\beta_{r}} \pi_{N}^{\frac{\alpha}{2},0} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta_{r}} \Phi^{k}\right), \upsilon_{N}\right) \\
= \left(\pi_{N}^{\frac{\alpha}{2},0} \sum_{r=0}^{m} q_{r} \left(D_{\tau}^{\beta_{r}} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta_{r}} \Phi^{k}\right), \upsilon_{N}\right) - \left(\sum_{r=0}^{m} q_{r} {}_{0}^{C} D_{t}^{\beta_{r}} \tilde{e}_{N}^{k}, \upsilon_{N}\right) \\
\stackrel{\Delta}{=} \mathcal{E}_{31}^{k} + \mathcal{E}_{32}^{k}, \qquad (2.25)$$

by combining the results of (2.3), the Hölder inequality, and the Young inequality, we have

$$\begin{aligned} \mathcal{E}_{31}^{k} &\leq \frac{\epsilon}{2} \sum_{r=0}^{m} q_{r} \left\| \pi_{N}^{\frac{\alpha}{2},0} \left(D_{\tau}^{\beta_{r}} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta_{r}} \Phi^{k} \right) \right\|^{2} + \frac{1}{2\epsilon} \| \upsilon_{N} \|^{2} \\ &\leq \frac{\epsilon}{2} C \sum_{r=0}^{m} q_{r} \left\| \left(D_{\tau}^{\beta_{r}} \Phi^{k} - {}_{0}^{C} D_{t}^{\beta_{r}} \Phi^{k} \right) \right\|^{2} + \frac{1}{2\epsilon} \| \upsilon_{N} \|^{2} \\ &\leq \frac{\epsilon}{2} C_{1,\Phi} \tau^{4-2\beta_{m}} + \frac{1}{2\epsilon} \| \upsilon_{N} \|^{2}, \end{aligned}$$

furthermore, according to Lemma 0.2, we have

$$\mathcal{E}_{32}^{k} \leq \frac{\epsilon}{2} C N^{\alpha - 2s} \sum_{r=0}^{m} q_{r} \left\| {}_{0}^{C} D_{t}^{\beta_{r}} \Phi \right\|_{s}^{2} + \frac{1}{2\epsilon} \left\| v_{N} \right\|^{2}.$$

Thus (2.25) becomes

$$\mathcal{E}_{3}^{k} \leq \frac{\epsilon}{2} C N^{\alpha - 2s} \sum_{r=0}^{m} q_{r} \left\| {}_{0}^{C} D_{t}^{\beta_{r}} \Phi \right\|_{s}^{2} + \frac{\epsilon}{2} C_{2,\Phi} \tau^{4 - 2\beta_{m}} + \frac{1}{\epsilon} \left\| v_{N} \right\|^{2}.$$
(2.26)

For the fourth term \mathcal{E}_4^k , it holds by invoking Remark 0.2

$$\mathcal{E}_{4}^{k} \leq \frac{\epsilon}{2} C N^{\alpha - 2r} \|\Phi\|_{s}^{2} + \frac{1}{2\epsilon} \|\upsilon_{N}\|^{2}.$$
(2.27)

Substituting (2.23), (2.24), (2.26) and (2.27) into (2.17), we can infer that

$$\left(\sum_{r=0}^{m} q_r D_{\tau}^{\beta_r} \hat{e}_N^k, \upsilon_N\right) + A\left(\hat{e}_N^k, \upsilon_N\right)$$

$$\leq \frac{5}{2\epsilon} \|\upsilon_N\|^2 + 4\epsilon CL^2 \|\hat{e}_N^{k-1}\|^2 + \epsilon CL^2 \|\hat{e}_N^{k-2}\|^2 + \frac{\epsilon}{2} CL^2 \|\hat{e}_N^{k-N_{\tilde{s}}}\|^2 + \tilde{\mathcal{R}}, \quad (2.28)$$

where

$$\tilde{\mathcal{R}} = \epsilon \tilde{C} N^{\alpha - 2s} \left(\sum_{r=0}^{m} q_r \left\| {}_{0}^{C} D_t^{\beta_r} \Phi \right\|_s^2 + \left\| \Phi \right\|_s^2 \right) + \epsilon \tilde{C} N^{-2r} \left\| \Phi \right\|_s^2 + \epsilon \tilde{C}_u \tau^{4 - 2\beta_m}.$$

Taking $v_N = \hat{e}_N^k$ in (2.28) and applying (22), we can conclude that

$$\sum_{r=0}^{m} \frac{q_r}{2} D_{\tau}^{\beta_r} \left\| \hat{e}_N^k \right\|^2 + \left\| \hat{e}_N^k \right\|_{\alpha/2}^2$$

$$\leq \frac{5}{2\epsilon} \left\| \hat{e}_N^k \right\|^2 + 4\epsilon C L^2 \left\| \hat{e}_N^{k-1} \right\|^2 + \epsilon C L^2 \left\| \hat{e}_N^{k-2} \right\|^2 + \frac{\epsilon}{2} C L^2 \left\| \hat{e}_N^{k-N_{\tilde{s}}} \right\|^2 + \tilde{\mathcal{R}},$$

namely,

$$\sum_{r=0}^{m} q_{r} D_{\tau}^{\beta_{r}} \left\| \hat{e}_{N}^{k} \right\|^{2} \leq \frac{5}{\epsilon} \left\| \hat{e}_{N}^{k} \right\|^{2} + 8\epsilon CL^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + 2\epsilon CL^{2} \left\| \hat{e}_{N}^{k-2} \right\|^{2} + \epsilon CL^{2} \left\| \hat{e}_{N}^{k-N_{\tilde{s}}} \right\|^{2} + \mathcal{R}_{N}^{k-1} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + \epsilon CL^{2} \left\| \hat{e}_{N}^{k-N_{\tilde{s}}} \right\|^{2} + \epsilon CL^{2} \left\| \hat{e}_{N}^{k-N_{\tilde{s}}$$

with $\mathcal{R} = 2\tilde{\mathcal{R}}$. By means of Lemma 0.12 and since $\epsilon > 0$, there exists a positive constant $\tau^* = \sqrt[\beta_m]{q_m}/{\left(2\Gamma(2-\beta_m)\frac{10}{\epsilon}\right)}$, when $\tau < \tau^*$, we have

$$\left\|\hat{e}_{N}^{k}\right\|^{2} \leq \frac{2\mathcal{R}t_{k}^{\beta_{m}}}{q_{m}\Gamma(1+\beta_{m})}E_{\beta_{m}}(2\mu t_{k}^{\beta_{m}}/q_{m}),$$

with $\mu = 10/\epsilon + 16\epsilon CL^2/(a_0^{\beta_m} - a_1^{\beta_m}) + 4C\epsilon L^2/(a_1^{\beta_m} - a_2^{\beta_m}) + 2C\epsilon L^2/(a_{N_{\bar{s}}-1}^{\beta_m} - a_{N_{\bar{s}}}^{\beta_m})$. Thus the scheme is unconditionally convergent. Finally, by means of triangle inequality and Lemma 0.2, we complete the proof of (2.15).

2.4 Numerical simulations

Here, we do some numerical experiments to clarify the convergence orders of the considered scheme in time and space. In addition, we show the impact of time and space fractional orders on the behavior of the dynamics for the solution of nonlinear delay reaction-diffusion equations. In order to investigate both temporal and spatial convergence orders independently, we'll calculate the orders of convergence in both of them using the L2-error norms (1.50).

Example 2.1. Consider nonlinear delay reaction-diffusion problem

$$\sum_{r=1}^{q} \frac{\partial^{\beta_r} \Phi}{\partial t^{\beta_r}}(x,t) = \frac{\partial^{\alpha} \Phi}{\partial |x|^{\alpha}}(x,t) - 2\Phi(x,t) + \frac{\Phi(x,t-1.5)}{1+\Phi^2(x,t-1.5)} + g(x,t), \quad x \in (0,1), \quad t \in (0,1],$$
(2.29)

where the fractional orders are chosen as $\beta_r = \frac{2q+r-5}{3q}$. The source function g(x,t) is given such that problem (2.29) has the exact solution $t^{\beta_5+1}x^2(1-x)^2$.

τ	$\alpha = 1.1$		$\alpha = 1.5$		$\alpha = 1.9$			
	Error	Order	Error	Order	Error	Order		
1.5/50	5.057×10^{-5}		4.692×10^{-5}		4.163×10^{-5}			
1.5/100	1.927×10^{-5}	1.392	1.989×10^{-5}	1.238	1.783×10^{-5}	1.223		
1.5/150	1.094×10^{-5}	1.395	1.192×10^{-5}	1.262	1.086×10^{-5}	1.224		
1.5/200	7.327×10^{-6}	1.396	8.283×10^{-6}	1.267	7.592×10^{-6}	1.244		
1.5/250	5.365×10^{-6}	1.396	6.226×10^{-6}	1.279	5.732×10^{-6}	1.259		
1.5/300	4.159×10^{-6}	1.397	4.933×10^{-6}	1.277	4.560×10^{-6}	1.255		
$2-\beta_5$		1.333		1.333		1.333		

Table 3: The L^2 -errors and their convergence orders versus τ and α at N = 50 for example 2.1.

In Table 3, we list the L^2 -errors and corresponding convergence orders with $\alpha = 1.1, 1.5, 1.9, N = 50$ for q = 5. We can see that these results confirm the expected theoretical order convergence in time. The convergence orders in space are depicted for different values of α and β at M = 500 in Figure 2.1. All the convergence results are in agreement with the theoretical results.



Figure 2.1 — Convergence order in space direction for different values of α at $\tau = 1.5/300.$

Chapter 3 Numerical algorithm for a generalized form of Schnakenberg reaction-diffusion model with gene expression time delay

This chapter is regarded as one that provides a direct application of fractional diffusion equations along with their respective numerical solutions. For the first time in literature, we present the analysis and the numerical solution of the time-space fractional Schnakenberg reaction-diffusion model with a fixed time delay. This model is a natural system of autocatalysis, which often occurs in a variety of biological systems. The numerical solutions are obtained by constructing an efficient numerical algorithm to approximate Riesz-space and Caputo-time fractional derivatives. More precisely, the L1 approximation is applied to discretize the temporal Caputo fractional derivative, while the Legendre-Galerkin spectral method is used to approximate the spatial fractional operator. The described method is shown to be unconditionally stable, with a $2 - \beta$ convergent order in time and an exponential rate of convergence in space in case of the smoothness of the solution. The error estimates for the obtained solution are derived by applying a proper discrete fractional Grönwall inequality. Moreover, we offer numerical simulations that demonstrate a close match with the theoretical study to evaluate the efficacy of our methodology.

3.1 Introduction

3.1.1 Model History

Modelling complex biological processes is a rising field of research that is important in the modelling of infectious diseases as well as many other phenomena such as auto-catalytic chemical processes and environmental problems. Among these complex processes are the abilities of biological systems to automatically adjust and maintain various physiological and other biologic parameters at a relatively constant level, known as Cellular self-regulation. This process occurs in many different areas of biology in clear order. Examples include cell distribution during embryonic development, cancerous tissue growth [157], vertebrate limb development [158], and animal skin patterning (eg, spots in tigers [159], feathers in birds [160]). The reason behind that is the ability of cells to differentiate according to their location in time and space is central to the evolution of shape. In addition, the concentration of a particular chemical morphogen or the concentration gradient of a particular morphogen across a cell's spatial domain influences the mechanisms of cell differentiation, such that cells are associated with the concentration of a particular morphogen to which they are exposed [161]. Differential gene expression is a mechanism by which cells can change their behaviour in response to their environment. This happens through cell-to-cell communication, which is mediated by cell signalling. The morphogen can describe this mechanism, which is considered a key concept in developmental biology [162; 163]. The Schnakenberg model uses the spatial distribution of morphogens' periodic oscillations to represent the intricate autocatalytic chemical reaction. This information can aid our understanding of how numerous morphogens interact with biological cells for generating patterns. Physically speaking, the Schnakenberg kinetics are obtained as one of eleven sets of kinetics that showed the prerequisites for limit cycle behavior, namely that the system requires at least three processes, one of which must be an autocatalytic [21; 164; 165]. These three processes are related by a simple equation to characterize this unrestrained catalytic chemical reaction, as follows

$$\emptyset_1 \xrightarrow[\ell_{-1}]{\ell_1} U, \quad \emptyset_2 \xrightarrow{\ell_2} V, \quad 2U + V \xrightarrow{\ell_3} U,$$
(3.1)

where U and V are the concentrations of the reactants and ℓ_i denotes deterministic reaction rates. Also, the chemicals \emptyset_1 and \emptyset_2 in the aforementioned equation are assumed to be continuous supplies, and their development is not taken into account. Numerous phenomena are covered by practical applications of Schnakenberg's model. For instance morphogen's spatial distribution, interactions between various shapes and cells and patterns, and the impact of various geometries on the structure of organs and embryos [166]. However, the Schnakenberg model has not received much attention in the literature. The majority of studies concentrated on investigations of the Schnakenberg model without consideration of a temporal delay, including [167]. The inclusion of time delay in cellular patterning is critical in Schnackenberg's type models. This is because it can help to create coordinated variations in the expression of genes that control vertebrate somite development and hence create specific patterns of development for different body parts [168]. A system may shift from a stable to an unstable state due to a temporal delay, which can also result in areas of instability and bifurcation. Applying the time delay to the last nonlinear term of (3.1), as indicated in [165], results in the reaction represented by

$$\emptyset_1 \xrightarrow[\ell_{-1}]{\ell_{-1}} U, \quad \emptyset_2 \xrightarrow{\ell_2} V, \quad 2U + V \xrightarrow{\ell_3} W, \quad W \xrightarrow{delay} 3U.$$
(3.2)

The reaction describes the internalization of two motes of U and one mote of V, which are withdrawn from the process and turned into substance W. However, a reaction at a previous time results in the production of three motes of U. As yet, a few studies particularly reference the Schnakenberg model while considering the effects of time delay. A significant proportion of these works concentrated on identifying integer-order or time-fractional-order analytical, semi-analytical, as well as numerical solutions for the Schnakenberg system. In [24], Jiang et al. studied the delayed Schnakenberg diffusive model under Neumann boundary conditions. In that paper, they used characteristic equation analysis, the center manifold theorem, and normal form theory to examine the Turing bifurcation (instability), Hopf bifurcation, and Turing-Hopf bifurcation for a delayed diffusion Schnakenberg system. The Schnakenberg diffusive model with time delays was proposed by Yi et al. in [23]. The authors examined how delaying gene expression might further lessen the possibility of outcomes formed, offering a justification for understanding how physiological self-organization systems behave when bifurcations take place. For the Schnakenberg system with gene-expression time delays, Alfifi [25] investigated analytical and numerical solutions. The author also discussed how diffusion and delays affect stability regions and bifurcation diagrams. It is worth noting that relatively few studies have examined the existence and uniqueness of solutions to the coupled reaction-diffusion Schnakenberg models with integer order derivatives. Among these efforts in this direction may be found in the references [169–171].

In light of these observations, this chapter contributes to the literature by developing a linearized explicit finite difference/spectral Galerkin method to the nonlinear time-space fractional Schnakenberg reaction-diffusion model with a time delay effect and then discussing its stability and convergence rate.

3.1.2 Mathematical model formulation

The nonlinear delayed fractional Schnakenberg model can be expressed in a general form by considering Φ_1 and Φ_2 as the concentrations of U and V in (3.2), respectively, and allowing the reactants to diffuse. Consequently, we have the following nonlinear system of delayed fractional diffusion equations:

$$\begin{cases}
\frac{\partial^{\beta} \Phi_{1}}{\partial t^{\beta}} - \kappa_{1} \frac{\partial^{\alpha} \Phi_{1}}{\partial |x|^{\alpha}} = f_{1} \left(\Phi_{1}(x,t), \Phi_{1}(x,t-s), \Phi_{2}(x,t), \Phi_{2}(x,t-s) \right) \\
+ g_{1}(x,t), \quad x \in \Omega, \quad t \in I, \\
\frac{\partial^{\beta} \Phi_{2}}{\partial t^{\beta}} - \kappa_{2} \frac{\partial^{\alpha} \Phi_{2}}{\partial |x|^{\alpha}} = f_{2} \left(\Phi_{1}(x,t), \Phi_{1}(x,t-s), \Phi_{2}(x,t), \Phi_{2}(x,t-s) \right) \\
+ g_{2}(x,t), \quad x \in \Omega, \quad t \in I, \\
\Phi_{j}(a,t) = \Phi_{j}(b,t) = 0, \quad j \in \{1,2\}, \quad t \in I, \\
\Phi_{1}(x,t) = \psi_{1}(x), \quad \Phi_{2}(x,t) = \psi_{2}(x), \quad x \in \Omega, \quad t \in [-s,0].
\end{cases}$$
(3.3)

Here, space and time domains are represented by $\Omega = [a, b] \subset \mathbb{R}$ and $I = [0,T] \subset \mathbb{R}$, respectively. $0 < \beta < 1$ is the fractional order of time in which the time-fractional derivative is considered in the sense of Caputo, whereas $1 < \alpha < 2$ is the fractional order of space. The autocatalyst and reactant, or activator and inhibitor, concentrations are represented by the two functions $\Phi_1(x,t)$ and $\Phi_2(x,t)$, respectively, at time t. The diffusion parameters of the two chemical concentrations are denoted by κ_1 and κ_2 . The temporal delay resulting from gene expression is represented by the positive constant s. Also, $g_1(x,t)$ and $g_2(x,t)$ are two known source functions. Additionally, to provide physically realistic interpretations whenever the time is somewhere between the delay point and zero, the initial conditions $\psi_1(x)$ and $\psi_2(x)$ have been selected as positive initial concentrations.

3.2 Derivation of Numerical Scheme

This section is devoted to constructing a linearized numerical approximation for the model system (3.3) based on combining L1 interpolation formula and the Legendre-Galerkin spectral method in order to discretize the temporal and space–fractional derivatives, respectively. We begin with temporal discretization and then detail the suggested scheme's spatial discretization.

3.2.1 Temporal discretization

We choose a time step given by $\tau = \frac{s}{N_s}$, where N_s is a positive integer, in order to uniformly divide the temporal domain I. This defines a class of uniform partitions denote by $t_n = n\tau$, for each $-N_s \leq n \leq M$, where $M = \lceil \frac{T}{\tau} \rceil$. Denote $\Phi_j^n = \Phi_j(., t_n), j \in (1, 2)$, then the following expressions can be used to get the L1estimate for the Caputo-time fractional derivative (6) of order $0 < \beta < 1$ at the time t_n , as [91]

$$\frac{\partial^{\beta} \Phi_{j}(x,t)}{\partial t^{\beta}}\Big|_{t=t_{n}} = \int_{0}^{t_{n}} \Phi_{j}'(x,\eta) \omega_{1-\beta}(t_{n}-\eta) d\eta
= \frac{1}{\Gamma(1-\beta)} \sum_{i=1}^{n} \frac{\Phi_{j}(x,t_{i}) - \Phi_{j}(x,t_{i-1})}{\tau} \int_{t_{i-1}}^{t_{i}} (t_{n}-\eta)^{-\beta} d\eta + r_{\tau}^{n}
= \frac{1}{\tau^{\beta} \Gamma(2-\beta)} \sum_{i=1}^{n} a_{n-i} \left(\Phi_{j}(x,t_{i}) - \Phi_{j}(x,t_{i-1})\right) + r_{\tau}^{n},$$
(3.4)

where the kernel $\omega_{\beta}(t) = \frac{t^{\beta-1}}{\Gamma(\beta)}$, for all t > 0. Also, for each $\varrho \ge 0$ the coefficients a_{ϱ} satisfy $a_{\varrho} = (\varrho + 1)^{1-\beta} - \varrho^{1-\beta}$. For each $n = 0, 1, \ldots, M$, if the function $\Phi_j \in C^2([0,T]; L^2(\Omega))$, then there is a positive constant C > 0 which means that the truncation error meets $||r_{\tau}^n|| \le C\tau^{2-\beta}$, (see [68]).

Definition 3.1. Let $\{\Phi_j^n\}_{n=0}^M$, $j \in (1,2)$ be a given sequence of real functions, then we can define the discrete time-fractional difference operator D_{τ}^{β} as follow [91]

$$D^{\beta}_{\tau}\Phi^{n}_{j} = \frac{\tau^{-\beta}}{\Gamma(2-\beta)} \sum_{i=1}^{n} a_{n-i} \ \delta_{t}\Phi^{i}_{j} = \frac{\tau^{-\beta}}{\Gamma(2-\beta)} \sum_{i=0}^{n} b_{n-i}\Phi^{i}_{j}, \quad \forall n = 1, \dots, M.$$
(3.5)

In the above formula, the constants are determined by $b_0 = a_0$, $b_n = -a_{n-1}$, $b_{n-i} = a_{n-i} - a_{n-i-1}$, $\forall 1 \le i \le n-1$, and also we define $\delta_t \Phi_j^i = \Phi_j^i - \Phi_j^{i-1}$.

Following that, at each time t_n , we shall present a semi-discretized version of the system (3.3). To this end, the formula (3.5) is used to estimate the time-fractional component, and Taylor's approximations are used to discretize the nonlinear source term. Thus, the resulting discrete-time system is as follows:

$$\begin{pmatrix}
D_{\tau}^{\beta}\Phi_{1}^{n} - \kappa_{1}\frac{\partial^{\alpha}\Phi_{1}^{n}}{\partial|x|^{\alpha}} = f_{1}\left(2\Phi_{1}^{n-1} - \Phi_{1}^{n-2}, \Phi_{1}^{n-N_{s}}, 2\Phi_{2}^{n-1} - \Phi_{2}^{n-2}, \Phi_{2}^{n-N_{s}}\right) \\
+g_{1}^{n}(x), \quad 1 \leq n \leq M, \\
D_{\tau}^{\beta}\Phi_{2}^{n} - \kappa_{2}\frac{\partial^{\alpha}\Phi_{2}^{n}}{\partial|x|^{\alpha}} = f_{2}\left(2\Phi_{1}^{n-1} - \Phi_{1}^{n-2}, \Phi_{1}^{n-N_{s}}, 2\Phi_{2}^{n-1} - \Phi_{2}^{n-2}, \Phi_{2}^{n-N_{s}}\right) \\
+g_{2}^{n}(x), \quad 1 \leq n \leq M, \\
\langle \Phi_{1}^{n}(x) = \psi_{1}(x), \quad \Phi_{2}^{n}(x) = \psi_{2}(x), \quad -N_{s} \leq n \leq 0, \quad x \in \Omega.
\end{cases}$$
(3.6)

Let us consider the coefficient $\lambda := \Gamma(2 - \beta)\tau^{\beta}$. Thus, this permits the recasting of the semi-scheme (3.6) into the analogous form given below:

$$\begin{cases} \Phi_{1}^{n} - \lambda \kappa_{1} \frac{\partial^{\alpha} \Phi_{1}^{n}}{\partial |x|^{\alpha}} = a_{n-1} \Phi_{1}^{0} - \sum_{i=1}^{n-1} b_{n-i} \Phi_{1}^{i} \\ + \lambda f_{1} \left(2\Phi_{1}^{n-1} - \Phi_{1}^{n-2}, \Phi_{1}^{n-N_{s}}, 2\Phi_{2}^{n-1} - \Phi_{2}^{n-2}, \Phi_{2}^{n-N_{s}} \right) + \lambda g_{1}^{n}(x), \quad 1 \le n \le M, \\ \Phi_{2}^{n} - \lambda \kappa_{2} \frac{\partial^{\alpha} \Phi_{2}^{n}}{\partial |x|^{\alpha}} = a_{n-1} \Phi_{2}^{0} - \sum_{i=1}^{n-1} b_{n-i} \Phi_{2}^{i} \\ + \lambda f_{2} \left(2\Phi_{1}^{n-1} - \Phi_{1}^{n-2}, \Phi_{1}^{n-N_{s}}, 2\Phi_{2}^{n-1} - \Phi_{2}^{n-2}, \Phi_{2}^{n-N_{s}} \right) + \lambda g_{2}^{n}(x), \quad 1 \le n \le M. \end{cases}$$

$$(3.7)$$

3.2.2 Spatial discretization

We first introduce the space function below to give suitable base functions that precisely meet the boundary requirements specified in spectral techniques for space-fractional differential equations in order to discretize the space-fractional derivatives[118; 133]:

$$\mathcal{W}_N^0 = \mathcal{P}_N(\Omega) \cap H_0^1(\Omega) = \operatorname{span} \left\{ \varphi_n(x) : n = 0, 1, \dots, N - 2 \right\}.$$
(3.8)

The function φ_n is defined as follows :

$$\varphi_n(x) = L_n(\hat{x}) - L_{n+2}(\hat{x}) = \frac{2n+3}{2(n+1)}(1-\hat{x}^2) \ J_n^{1,1}(\hat{x}), \quad \forall \ \hat{x} \in [-1,1], \quad (3.9)$$

where $x = \frac{1}{2}((b-a)\hat{x} + a + b) \in [a, b]$. Hence, the fully discrete *L*1-Galerkin spectral scheme for for the system model (3.3) consists of the set of approximations $\Phi_{j,N}^n \in \mathcal{W}_N^0$, $j \in (1, 2)$, such that $\forall v \in \mathcal{W}_N^0$, satisfying the following system

$$\begin{pmatrix}
\left(\Phi_{1,N}^{n}, \upsilon\right) - \lambda \kappa_{1} \left(\frac{\partial^{\alpha}}{\partial |x|^{\alpha}} \Phi_{1,N}^{n}, \upsilon\right) = a_{n-1} \left(\Phi_{1,N}^{0}, \upsilon\right) - \sum_{i=1}^{n-1} b_{n-i} \left(\Phi_{1,N}^{i}, \upsilon\right) \\
+ \lambda \left(I_{N} f_{1} \left(2\Phi_{1,N}^{n-1} - \Phi_{1,N}^{n-2}, \Phi_{1,N}^{n-N_{s}}, 2\Phi_{2,N}^{n-1} - \Phi_{2,N}^{n-2}, \Phi_{2,N}^{n-N_{s}}\right), \upsilon\right) \\
+ \lambda I_{N} \left(g_{1}^{n}(x), \upsilon\right), \quad 1 \leq n \leq M, \\
\left(\Phi_{2,N}^{n}, \upsilon\right) - \lambda \kappa_{2} \left(\frac{\partial^{\alpha}}{\partial |x|^{\alpha}} \Phi_{2,N}^{n}, \upsilon\right) = a_{n-1} \left(\Phi_{2,N}^{0}, \upsilon\right) - \sum_{i=1}^{n-1} b_{n-i} \left(\Phi_{2,N}^{i}, \upsilon\right) \\
+ \lambda \left(I_{N} f_{2} \left(2\Phi_{1,N}^{n-1} - \Phi_{1,N}^{n-2}, \Phi_{1,N}^{n-N_{s}}, 2\Phi_{2,N}^{n-1} - \Phi_{2,N}^{n-2}, \Phi_{2,N}^{n-N_{s}}\right), \upsilon\right) \\
+ \lambda I_{N} \left(g_{2}^{n}(x), \upsilon\right), \quad 1 \leq n \leq M, \\
\Phi_{1,N}^{0} = \pi_{N}^{1,0} \psi_{1}(t_{n},x), \quad \Phi_{2,N}^{0} = \pi_{N}^{1,0} \psi_{2}(t_{n},x), \quad -N_{s} \leq n \leq 0,
\end{cases}$$
(3.10)

where $\pi_N^{1,0}$ is a suitable projection operator in this case. Following this, we could further generalize the approximation as

$$\Phi_{j,N}^n = \sum_{i=0}^{N-2} \hat{\Phi}_{j,i}^n \varphi_i(x), \quad j \in \{1,2\},$$
(3.11)

where $\hat{\Phi}_{j,i}^n$ are an undetermined expansion coefficients. The uniform full discrete scheme for the model (3.3) can be expressed as a linear system in a matrix form using (3.11), Lemma 0.1 and allowing $v = \varphi_k$, for each $0 \le k \le N - 2$ as follows:

$$\left(\bar{M} - \lambda c_{\alpha}(S + S^{T})\right) U_{j}^{n} = K_{j}^{n-1} + \lambda H_{j}^{n-1} + \lambda G_{j}^{n}, \quad j \in \{1, 2\},$$
(3.12)

where the following provides the notations in expression (3.12):

$$s_{ij} = \int_{\Omega} {}_{a} D_{x}^{\frac{\alpha}{2}} \varphi_{i}(x)_{x} D_{b}^{\frac{\alpha}{2}} \varphi_{j}(x) dx, \qquad S = (s_{ij})_{i,j=0}^{N-2},$$

$$m_{ij} = \int_{\Omega} \varphi_{i}(x) \varphi_{j}(x) dx, \qquad \bar{M} = (m_{ij})_{i,j=0}^{N-2}, \qquad K^{n-1} = -\sum_{i=0}^{n-1} b_{n-i} \bar{M} U_{j}^{i},$$

$$h_{j,i}^{n-1} = \int_{\Omega} \varphi_{i}(x) I_{N} f_{j} \left(2\Phi_{1,N}^{n-1} - \Phi_{1,N}^{n-2}, \Phi_{1,N}^{n-N_{s}}, 2\Phi_{2,N}^{n-1} - \Phi_{2,N}^{n-2}, \Phi_{2,N}^{n-N_{s}} \right) dx,$$

$$H_{j}^{n-1} = (h_{j,0}^{n-1}, h_{j,1}^{n-1}, \dots, h_{j,N-2}^{n-1})^{\top}, \qquad U_{j}^{n} = (\hat{\Phi}_{j,0}^{n}, \hat{\Phi}_{j,1}^{n}, \dots, \hat{\Phi}_{j,N-2}^{n})^{\top},$$

$$g_{j,i}^{n} = \int_{\Omega} \varphi_{i}(x) I_{N} g_{j}^{n} dx, \qquad G_{j}^{n} = (g_{j,0}^{n}, g_{j,1}^{n}, \dots, g_{j,N-2}^{n})^{\top}. \qquad (3.13)$$

Moreover, the elements of the stiffness matrix S and the mass matrix \overline{M} can be easily calculated using lemma 1.1.

3.3 Theoretical analysis

This section aims to verify how effectively the numerical solution of the suggested approach for the model (3.3). We start with stability analysis and give the theorem of stability in the first subsection. The second subsection is devoted to the convergence analysis and the theorem of convergence is given there. We assume that the Lipschitz condition below holds for the function f_j , $j \in (1, 2)$, which is necessary for the theoretical analysis, i.e,

$$|f_j(\Phi_1, v_1) - f_j(\Phi_2, v_2)| \le L \left(|\Phi_1 - \Phi_2| + |v_1 - v_2| \right), \quad j \in (1, 2), \tag{3.14}$$

where L is a positive constant.

3.3.1 Stability analysis

The week formulation of the proposed scheme can be expressed as: find $\{\Phi_{j,N}^k\}_{k=1}^M \in \mathcal{P}_N, j \in \{1,2\}$ such that for every $\upsilon_N \in \mathcal{P}_N$, satisfying the follow-

ing

$$(D_{\tau}^{\beta} \Phi_{j,N}^{k}, \upsilon_{N}) + A (\Phi_{j,N}^{k}, \upsilon_{N})$$

$$= (I_{N} f_{j} (2\Phi_{1,N}^{k-1} - \Phi_{1,N}^{k-2}, \Phi_{1,N}^{k-N_{s}}, 2\Phi_{2,N}^{k-1} - \Phi_{2,N}^{k-2}, \Phi_{2,N}^{k-N_{s}}), \upsilon_{N}) + (I_{N} g_{j}^{k}, \upsilon_{N}),$$

$$(3.15)$$

with initial conditions

$$\Phi_{j,N}^{k} = \pi_{N}^{1,0} \varphi^{k}, \quad -N_{s} \le k \le 0.$$

Due to the linear iterative nature of the method, a solution to an algebraic equation system is all that is required at each iteration. The suggested scheme's well-posedness, meaning it is uniquely solvable and continues to rely on its initial boundary conditions which is sufficient to hold the Lax-Milgram lemma's assumptions [136]. In particular, it can be seen from equation (3.15) that the bilinear form $A(\cdot, \cdot)$ is continuous as well as it coercive in $H_0^{\alpha/2} \times H_0^{\alpha/2}$. We also assume that $\{\tilde{\Phi}_{j,N}^k\}_{k=1}^M \in \mathcal{P}_N, j \in \{1,2\}$ are the solutions of the following variational system form

$$\begin{pmatrix} D_{\tau}^{\beta} \tilde{\Phi}_{j,N}^{k}, \upsilon_{N} \end{pmatrix} + A \left(\tilde{\Phi}_{j,N}^{k}, \upsilon_{N} \right)$$

$$= \left(I_{N} f_{j} \left(2 \tilde{\Phi}_{1,N}^{k-1} - \tilde{\Phi}_{1,N}^{k-2}, \tilde{\Phi}_{1,N}^{k-N_{s}}, 2 \tilde{\Phi}_{2,N}^{k-1} - \tilde{\Phi}_{2,N}^{k-2}, \tilde{\Phi}_{2,N}^{k-N_{s}} \right), \upsilon_{N} \right) + \left(I_{N} \tilde{g}_{j}^{k}, \upsilon_{N} \right),$$

$$(3.16)$$

with initial conditions

$$\tilde{\Phi}_{j,N}^k = \pi_N^{1,0} \varphi^k, \ -N_s \le k \le 0, \quad j \in \{1,2\}.$$

Now, we are ready to offer the stability theorem in the context of the subsequent discussion.

Theorem 3.1. The suggested method (3.15) in this sense, is said to be unconditionally stable, which means it holds for $\tau > 0$,

$$\left\|\Phi_{1,N}^{k} - \tilde{\Phi}_{1,N}^{k}\right\|^{2} + \left\|\Phi_{2,N}^{k} - \tilde{\Phi}_{2,N}^{k}\right\|^{2} \le C \max_{1 \le k \le M} \left(\left\|g_{1}^{k} - \tilde{g}_{1}^{k}\right\|^{2} + \left\|g_{2}^{k} - \tilde{g}_{2}^{k}\right\|^{2}\right),$$

where C is a positive constant independent of N and τ .

Proof. Take $\rho_{1,N}^k = \Phi_{1,N}^k - \tilde{\Phi}_{1,N}^k$ and $\rho_{2,N}^k = \Phi_{2,N}^k - \tilde{\Phi}_{2,N}^k$. Subtracting (3.16) from (3.15) at j = 1, it holds

$$\begin{pmatrix} D_{\tau}^{\beta} \rho_{1,N}^{k}, \upsilon_{N} \end{pmatrix} + A \left(\rho_{1,N}^{k}, \upsilon_{N} \right)$$

$$= \begin{pmatrix} I_{N} f_{1} \left(2\Phi_{1,N}^{k-1} - \Phi_{1,N}^{k-2}, \Phi_{1,N}^{k-N_{s}}, 2\Phi_{2,N}^{k-1} - \Phi_{2,N}^{k-2}, \Phi_{2,N}^{k-N_{s}} \right) \\ - I_{N} f_{1} \left(2\tilde{\Phi}_{1,N}^{k-1} - \tilde{\Phi}_{1,N}^{k-2}, \tilde{\Phi}_{1,N}^{k-N_{s}}, 2\tilde{\Phi}_{2,N}^{k-1} - \tilde{\Phi}_{2,N}^{k-2}, \tilde{\Phi}_{2,N}^{k-N_{s}} \right), \upsilon_{N} \end{pmatrix} \\ + \begin{pmatrix} I_{N} g_{1}^{k} - I_{N} \tilde{g}_{1}^{k}, \upsilon_{N} \end{pmatrix}.$$

$$(3.17)$$

Applying the Lipschitz condition (3.14) and using Hölder inequality side by side to Young inequality, we derive the following for the first term of the right-hand side

$$\begin{split} & \left(I_{N} f_{1} \left(2\Phi_{1,N}^{k-1} - \Phi_{1,N}^{k-2}, \Phi_{1,N}^{k-N_{s}}, 2\Phi_{2,N}^{k-1} - \Phi_{2,N}^{k-2}, \Phi_{2,N}^{k-N_{s}}\right) \\ & - I_{N} f_{1} \left(2\tilde{\Phi}_{1,N}^{k-1} - \tilde{\Phi}_{1,N}^{k-2}, \tilde{\Phi}_{1,N}^{k-N_{s}}, 2\tilde{\Phi}_{2,N}^{k-1} - \tilde{\Phi}_{2,N}^{k-2}, \tilde{\Phi}_{2,N}^{k-N_{s}}\right), \upsilon_{N}\right) \\ & \leq C_{1} L_{1} \left(\left\|2\rho_{1,N}^{k-1} - \rho_{1,N}^{k-2}\right\| + \left\|\rho_{1,N}^{k-N_{s}}\right\| + \left\|2\rho_{2,N}^{k-1} - \rho_{2,N}^{k-2}\right\| + \left\|\rho_{2,N}^{k-N_{s}}\right\|\right) \|\upsilon_{N}\| \\ & \leq \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left\|2\rho_{1,N}^{k-1} - \rho_{1,N}^{k-2}\right\|^{2} + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left\|\rho_{1,N}^{k-N_{s}}\right\|^{2} + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left\|2\rho_{2,N}^{k-1} - \rho_{2,N}^{k-2}\right\|^{2} \\ & + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left\|\rho_{2,N}^{k-N_{s}}\right\|^{2} + \frac{1}{2\epsilon_{1}} \|\upsilon_{N}\|^{2} \\ & \leq 4\epsilon_{1}C_{1}L_{1}^{2} \left(\left\|\rho_{1,N}^{k-1}\right\|^{2} + \left\|\rho_{2,N}^{k-1}\right\|^{2}\right) + \epsilon_{1}C_{1}L_{1}^{2} \left(\left\|\rho_{1,N}^{k-2}\right\|^{2} + \left\|\rho_{2,N}^{k-2}\right\|^{2}\right) \\ & + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left(\left\|\rho_{1,N}^{k-N_{s}}\right\|^{2} + \left\|\rho_{2,N}^{k-N_{s}}\right\|^{2}\right) + \frac{1}{2\epsilon_{1}} \|\upsilon_{N}\|^{2}, \end{split}$$

and for the second term

$$(I_N g_1^k - I_N \tilde{g}_1^k, \upsilon_N) \le \frac{\epsilon_1}{2} C \|g_1^k - \tilde{g}_1^k\|^2 + \frac{1}{2\epsilon_1} \|\upsilon_N\|^2.$$

Then (3.17) becomes

$$\begin{aligned} & \left(D_{\tau}^{\beta} \rho_{1,N}^{k}, \upsilon_{N} \right) + A(\rho_{1,N}^{k}, \upsilon_{N}) \\ & \leq \frac{1}{\epsilon_{1}} \left\| \upsilon_{N} \right\|^{2} + 4\epsilon_{1}C_{1}L_{1}^{2} \left(\left\| \rho_{1,N}^{k-1} \right\|^{2} + \left\| \rho_{2,N}^{k-1} \right\|^{2} \right) + \epsilon_{1}C_{1}L_{1}^{2} \left(\left\| \rho_{1,N}^{k-2} \right\|^{2} + \left\| \rho_{2,N}^{k-2} \right\|^{2} \right) \\ & \quad + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left(\left\| \rho_{1,N}^{k-N_{s}} \right\|^{2} + \left\| \rho_{2,N}^{k-N_{s}} \right\|^{2} \right) + \frac{\epsilon_{1}}{2}C \left\| g_{1}^{k} - \tilde{g}_{1}^{k} \right\|^{2}. \end{aligned}$$
Taking $v_N = \rho_{1,N}^k$ and using (22) and (16), we can deduce that

$$\begin{split} &\frac{1}{2}D_{\tau}^{\beta} \left\|\rho_{1,N}^{k}\right\|^{2} + \left|\rho_{1}\right|_{\alpha/2}^{2} \\ &\leq \frac{1}{\epsilon_{1}} \left\|\upsilon_{N}\right\|^{2} + 4\epsilon_{1}C_{1}L_{1}^{2} \left(\left\|\rho_{1,N}^{k-1}\right\|^{2} + \left\|\rho_{2,N}^{k-1}\right\|^{2}\right) + \epsilon_{1}C_{1}L_{1}^{2} \left(\left\|\rho_{1,N}^{k-2}\right\|^{2} + \left\|\rho_{2,N}^{k-2}\right\|^{2}\right) \\ &+ \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left(\left\|\rho_{1,N}^{k-N_{s}}\right\|^{2} + \left\|\rho_{2,N}^{k-N_{s}}\right\|^{2}\right) + \frac{\epsilon_{1}}{2}C \left\|g_{1}^{k} - \tilde{g}_{1}^{k}\right\|^{2}, \end{split}$$

namely,

$$D_{\tau}^{\beta} \left\| \rho_{1,N}^{k} \right\|^{2} \leq \frac{2}{\epsilon_{1}} \left\| \rho_{1,N}^{k} \right\|^{2} + 8\epsilon_{1}C_{1}L_{1}^{2} \left(\left\| \rho_{1,N}^{k-1} \right\|^{2} + \left\| \rho_{2,N}^{k-1} \right\|^{2} \right) + 2\epsilon_{1}C_{1}L_{1}^{2} \left(\left\| \rho_{1,N}^{k-2} \right\|^{2} + \left\| \rho_{2,N}^{k-2} \right\|^{2} \right) + \epsilon_{1}C_{1}L_{1}^{2} \left(\left\| \rho_{1,N}^{k-N_{s}} \right\|^{2} + \left\| \rho_{2,N}^{k-N_{s}} \right\|^{2} \right) + \epsilon_{1}C_{1} \left\| g_{1}^{k} - \tilde{g}_{1}^{k} \right\|^{2}.$$

$$(3.18)$$

The same steps can be used to arrive at the same conclusion for (3.15) and (3.16) at j = 2, i.e.,

$$D_{\tau}^{\beta} \|\rho_{2,N}^{k}\|^{2} \leq \frac{2}{\epsilon_{2}} \|\rho_{2,N}^{k}\|^{2} + 8\epsilon_{2}C_{2}L_{2}^{2} \left(\|\rho_{1,N}^{k-1}\|^{2} + \|\rho_{2,N}^{k-1}\|^{2}\right) + 2\epsilon_{2}C_{2}L_{2}^{2} \left(\|\rho_{1,N}^{k-2}\|^{2} + \|\rho_{2,N}^{k-2}\|^{2}\right) + \epsilon_{2}C_{2}L_{2}^{2} \left(\|\rho_{1,N}^{k-N_{s}}\|^{2} + \|\rho_{2,N}^{k-N_{s}}\|^{2}\right) + \epsilon_{2}C_{2} \|g_{2}^{k} - \tilde{g}_{2}^{k}\|^{2}.$$

$$(3.19)$$

Adding (3.18) and (3.19) together, we obtain

$$\begin{aligned} D_{\tau}^{\beta} \left(\left\| \rho_{1,N}^{k} \right\|^{2} + \left\| \rho_{2,N}^{k} \right\|^{2} \right) \\ &\leq \frac{4}{\min\{\epsilon_{1},\epsilon_{2}\}} \left(\left\| \rho_{1,N}^{k} \right\|^{2} + \left\| \rho_{2,N}^{k} \right\|^{2} \right) + 16\tilde{C} \left(\left\| \rho_{1,N}^{k-1} \right\|^{2} + \left\| \rho_{2,N}^{k-1} \right\|^{2} \right) \\ &+ 4\tilde{C} \left(\left\| \rho_{1,N}^{k-2} \right\|^{2} + \left\| \rho_{2,N}^{k-2} \right\|^{2} \right) + 2\tilde{C} \left(\left\| \rho_{1,N}^{k-N_{s}} \right\|^{2} + \left\| \rho_{2,N}^{k-N_{s}} \right\|^{2} \right) \\ &+ \hat{C} \left(\left\| g_{1}^{k} - \tilde{g}_{1}^{k} \right\|^{2} + \left\| g_{2}^{k} - \tilde{g}_{2}^{k} \right\|^{2} \right), \end{aligned}$$

where $\tilde{C} = \max\{\epsilon_1 C_1 L_1^2, \epsilon_2 C_2 L_2^2\}$ and $\hat{C} = \max\{\epsilon_1 C_1, \epsilon_2 C_2\}$. A direct application of the Grönwall inequality (see Lemma 0.11) and since $\min\{\epsilon_1, \epsilon_2\} > 0$, there exists

a positive constant $\tau^* = \sqrt[\beta]{1/(2\Gamma(2-\beta) \frac{4}{\min\{\epsilon_1,\epsilon_2\}})}$, when $\tau < \tau^*$, we have

$$\left\|\rho_{1,N}^{k}\right\|^{2} + \left\|\rho_{2,N}^{k}\right\|^{2} \leq \frac{2\epsilon C t_{k}^{\beta}}{\Gamma(1+\beta)} E_{\beta}\left(2\mu t_{k}^{\beta}\right) \max_{1\leq k\leq M}\left(\left\|g_{1}^{k}-\tilde{g}_{1}^{k}\right\|^{2} + \left\|g_{2}^{k}-\tilde{g}_{2}^{k}\right\|^{2}\right),$$

with $\mu = \frac{4}{\min\{\epsilon_1, \epsilon_2\}} + 16\tilde{C}/(a_0 - a_1) + 4\tilde{C}/(a_1 - a_2) + 2\tilde{C}/(a_{N_s-1} - a_{N_s})$. Therefore, the proposed method is guaranteed to be unconditionally stable.

3.3.2 Convergence

Here, we present the proof of the convergence theorem for the suggested scheme (3.15) using discrete error estimates.

Theorem 3.2. Let $\{\Phi_j^k\}_{k=-N_s}^M$ and $\{\Phi_{j,N}^k\}_{k=-N_s}^M$, $j \in \{1,2\}$ be the exact and the approximate solutions of the model system (3.3) and the proposed method (3.15), respectively. Assume that $\Phi_j \in C^2([0,T]; L^2(\Omega)) \cap C^1([0,T]; H^s(\Omega))$. Then for a positive constant C independent of N and τ , the following statement is valid

$$\left|\Phi_{1}^{k}-\Phi_{1,N}^{k}\right|_{\alpha/2}+\left|\Phi_{2}^{k}-\Phi_{2,N}^{k}\right|_{\alpha/2}\leq C\left(N^{\alpha/2-s}+N^{-r}+\tau^{2-\beta}\right),\quad 1\leq k\leq M,$$
(3.20)

where r denotes the regularity parameter of the source term.

Proof. Take $\Phi_j^k - \Phi_{j,N}^k = e_{j,N}^k = \left(\Phi_j^k - \pi_N^{\frac{\alpha}{2},0}\Phi_j^k\right) + \left(\pi_N^{\frac{\alpha}{2},0}\Phi_j^k - \Phi_{j,N}^k\right) \stackrel{\Delta}{=} \tilde{e}_{j,N}^k + \hat{e}_{j,N}^k$. The system (3.3) has the following weak formulation:

$$\begin{pmatrix} {}^{C}_{0}D^{\beta}_{t}\Phi^{k}_{j}, \upsilon_{N} \end{pmatrix} + A\left(\Phi^{k}_{j}, \upsilon_{N}\right) = \left(f_{j}\left(\Phi^{k}_{1}, \Phi^{k-N_{s}}_{1}, \Phi^{k}_{2}, \Phi^{k-N_{s}}_{2}\right), \upsilon_{N}\right) + \left(g^{k}_{j}, \upsilon_{N}\right).$$

$$(3.21)$$

By subtracting (3.15) from (3.21), and using the notion of orthogonal projection, then the error equation at j = 1, fulfills

$$(D^{\beta}_{\tau} \ \hat{e}^{k}_{1,N}, \ \upsilon_{N}) + A(\hat{e}^{k}_{1,N}, \upsilon_{N}) \stackrel{\Delta}{=} \mathcal{E}^{k}_{1} + \mathcal{E}^{k}_{2} + \mathcal{E}^{k}_{3} + +\mathcal{E}^{k}_{4}, \qquad (3.22)$$

where

$$\begin{split} \mathcal{E}_{1}^{k} &= \left(I_{N} f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) \\ &- I_{N} f_{1} \left(2\Phi_{1,N}^{k-1} - \Phi_{1,N}^{k-2}, \Phi_{1,N}^{k-N_{s}}, 2\Phi_{2,N}^{k-1} - \Phi_{2,N}^{k-2}, \Phi_{2,N}^{k-N_{s}} \right), \upsilon_{N} \right), \\ \mathcal{E}_{2}^{k} &= \left(f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) - I_{N} f_{j} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right), \upsilon_{N} \right), \\ \mathcal{E}_{3}^{k} &= \left(D_{\tau}^{\beta} \pi_{N}^{\frac{\alpha}{2},0} \Phi_{1}^{k} - {}_{0}^{C} D_{t}^{\beta} \Phi_{1}^{k}, \upsilon_{N} \right), \\ \mathcal{E}_{4}^{k} &= \left(g_{j}^{k} - I_{N} g_{j}^{k}, \upsilon_{N} \right). \end{split}$$

To proceed, we make an estimate of the terms \mathcal{E}_1^k , \mathcal{E}_2^k , \mathcal{E}_3^k and \mathcal{E}_4^k on the right-hand side. Regarding the first term \mathcal{E}_1^k , we can write it as

$$\mathcal{E}_1^k \stackrel{\Delta}{=} \mathcal{E}_{11}^k + \mathcal{E}_{12}^k, \tag{3.23}$$

where

$$\begin{aligned} \mathcal{E}_{11}^{k} &= \left(I_{N} f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) \\ &- I_{N} f_{1} \left(2\Phi_{1}^{k-1} - \Phi_{1}^{k-2}, \Phi_{1}^{k-N_{s}}, 2\Phi_{2}^{k-1} - \Phi_{2}^{k-2}, \Phi_{2}^{k-N_{s}} \right), \upsilon_{N} \right), \\ \mathcal{E}_{12}^{k} &= \left(I_{N} f_{1} \left(2\Phi_{1}^{k-1} - \Phi_{1}^{k-2}, \Phi_{1}^{k-N_{s}}, 2\Phi_{2}^{k-1} - \Phi_{2}^{k-2}, \Phi_{2}^{k-N_{s}} \right) \\ &- I_{N} f_{1} \left(2\Phi_{1,N}^{k-1} - \Phi_{1,N}^{k-2}, \Phi_{1,N}^{k-N_{s}}, 2\Phi_{2,N}^{k-1} - \Phi_{2,N}^{k-2}, \Phi_{2,N}^{k-N_{s}} \right), \upsilon_{N} \right). \end{aligned}$$

Invoking Taylor expansion holds

$$f_1\left(\Phi_1^k, \Phi_1^{k-N_s}, \Phi_2^k, \Phi_2^{k-N_s}\right) = f_1\left(2\Phi_1^{k-1} - \Phi_1^{k-2}, \Phi_1^{k-N_s}, 2\Phi_2^{k-1} - \Phi_2^{k-2}, \Phi_2^{k-N_s}\right) + \tilde{c}_{\Phi}\tau^2.$$

In addition, we use Hölder's and Young's inequalities to

$$\mathcal{E}_{11}^{k} \leq \left\| I_{N} f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) - I_{N} f_{1} \left(2\Phi_{1}^{k-1} - \Phi_{1}^{k-2}, \Phi_{1}^{k-N_{s}}, 2\Phi_{2}^{k-1} - \Phi_{2}^{k-2}, \Phi_{2}^{k-N_{s}} \right) \right\| \| v_{N} \| \\
\leq C_{1} \left\| f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) - f_{1} \left(2\Phi_{1}^{k-1} - \Phi_{1}^{k-2}, \Phi_{1}^{k-N_{s}}, 2\Phi_{2}^{k-1} - \Phi_{2}^{k-2}, \Phi_{2}^{k-N_{s}} \right) \right\| \| v_{N} \| \\
\leq \frac{\epsilon_{1}}{2} C_{1} \tilde{c}_{\Phi} \tau^{4} + \frac{1}{2\epsilon_{1}} \| v_{N} \|^{2}.$$
(3.24)

Invoking the Lipschitz condition (3.14) and using Hölder inequality side by side to Young inequality, we deduce that

$$\begin{aligned} \mathcal{E}_{12}^{k} &\leq L_{1}C_{1}\left(\left\|2e_{1,N}^{k-1} - e_{1,N}^{k-2}\right\| + \left\|e_{1,N}^{k-N_{s}}\right\| + \left\|2e_{2,N}^{k-1} - e_{2,N}^{k-2}\right\| + \left\|e_{2,N}^{k-N_{s}}\right\|\right) \|\upsilon_{N}\| \\ &\leq \frac{\epsilon_{1}}{2}L_{1}C_{1}\left(\left\|2\hat{e}_{1,N}^{k-1} - \hat{e}_{1,N}^{k-2}\right\| + \left\|\hat{e}_{1,N}^{k-N_{s}}\right\| + \left\|2\hat{e}_{2,N}^{k-1} - \hat{e}_{2,N}^{k-2}\right\| + \left\|\hat{e}_{2,N}^{k-N_{s}}\right\| \\ &+ \left\|2\tilde{e}_{1,N}^{k-1} - \tilde{e}_{1,N}^{k-2}\right\| + \left\|\hat{e}_{1,N}^{k-N_{s}}\right\| + \left\|2\tilde{e}_{2,N}^{k-1} - \tilde{e}_{2,N}^{k-2}\right\| + \left\|\hat{e}_{2,N}^{k-N_{s}}\right\|\right)^{2} + \frac{1}{2\epsilon_{1}}\|\upsilon_{N}\|^{2} \\ &\leq \frac{8\epsilon_{1}}{2}C_{1}L_{1}^{2}\left(\left\|\hat{e}_{1,N}^{k-1}\right\|^{2} + \left\|\hat{e}_{2,N}^{k-1}\right\|^{2}\right) + \frac{2\epsilon}{2}CL^{2}\left(\left\|\hat{e}_{1,N}^{k-2}\right\|^{2} + \left\|\hat{e}_{2,N}^{k-2}\right\|^{2}\right) \\ &+ \frac{\epsilon}{2}CL^{2}\left(\left\|\hat{e}_{1,N}^{k-N_{s}}\right\|^{2} + \left\|\hat{e}_{2,N}^{k-N_{s}}\right\|^{2}\right) + \frac{8\epsilon_{1}}{2}C_{1}L_{1}^{2}\left(\left\|\tilde{e}_{1,N}^{k-1}\right\|^{2} + \left\|\tilde{e}_{2,N}^{k-1}\right\|^{2}\right) \\ &+ \frac{2\epsilon_{1}}{2}C_{1}L_{1}^{2}\left(\left\|\hat{e}_{1,N}^{k-2}\right\|^{2} + \left\|\tilde{e}_{2,N}^{k-2}\right\|^{2}\right) + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2}\left(\left\|\tilde{e}_{1,N}^{k-1}\right\|^{2} + \left\|\tilde{e}_{2,N}^{k-1}\right\|^{2}\right) \\ &+ \frac{1}{2\epsilon_{1}}\|\upsilon_{N}\|^{2}. \end{aligned}$$

$$(3.25)$$

In addition, considering the Lemmas 0.2 and 0.3, it can be shown that

$$\begin{split} \left\| \tilde{e}_{1,N}^{k-1} \right\|^2 &\leq \frac{C}{C_1} N^{\alpha - 2s} \left\| \Phi_1^{k-1} \right\|_s^2, \\ \left\| \tilde{e}_{1,N}^{k-2} \right\|^2 &\leq \frac{C}{C_1} N^{\alpha - 2s} \left\| \Phi_1^{k-2} \right\|_s^2, \\ \left\| \tilde{e}_{1,N}^{k-N_s} \right\|^2 &\leq \frac{C}{C_1} N^{\alpha - 2s} \left\| \Phi_1^{k-n} \right\|_s^2, \end{split}$$

then (3.25) becomes

$$\mathcal{E}_{12}^{k} \leq 4\epsilon_{1}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-1} \right\|^{2} + \epsilon_{1}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-2} \right\|^{2} + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-N_{s}} \right\|^{2} + \tilde{C}_{1}N^{\alpha-2s} \left\| \Phi_{1} \right\|_{s}^{2} + \frac{1}{2\epsilon_{1}} \left\| v_{N} \right\|^{2}.$$

$$(3.26)$$

Substituting (3.24) and (3.26) into (3.23), we obtain that

$$\mathcal{E}_{1}^{k} \leq \frac{1}{\epsilon_{1}} \left\| v_{N} \right\|^{2} + 4\epsilon_{1}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-1} \right\|^{2} + \epsilon_{1}C_{1} \left\| \hat{e}_{1,N}^{k-2} \right\|^{2} + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-N_{s}} \right\|^{2} + \tilde{C}_{1}N^{\alpha-2s} \left\| \Phi \right\|_{s}^{2} + \frac{\epsilon_{1}}{2}\tilde{c}_{\Phi}\tau^{4}.$$
(3.27)

Hölder's inequality, Young's inequality, and Lemma 0.5 allow us to deduce the following for the second term \mathcal{E}_2^k as follows:

$$\mathcal{E}_{2}^{k} \leq \left\| f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) - I_{N} f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) \right\| \|\upsilon_{N}\| \\ \leq \frac{\epsilon_{1}}{2} \left\| f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) - I_{N} f_{1} \left(\Phi_{1}^{k}, \Phi_{1}^{k-N_{s}}, \Phi_{2}^{k}, \Phi_{2}^{k-N_{s}} \right) \right\|^{2} + \frac{1}{2\epsilon_{1}} \|\upsilon_{N}\|^{2} \\ \leq \frac{1}{2\epsilon_{1}} \|\upsilon_{N}\|^{2} + \frac{\epsilon_{1}}{2} C_{1} N^{-2r} \|\Phi_{1}\|_{s}, \qquad (3.28)$$

For the third term \mathcal{E}_3^k , it holds

$$\mathcal{E}_{3}^{k} = \left(D_{\tau}^{\beta} \pi_{N}^{\frac{\alpha}{2},0} \Phi_{1}^{k} - {}_{0}^{C} D_{t}^{\beta} \pi_{N}^{\frac{\alpha}{2},0} \Phi_{1}^{k}, \upsilon_{N} \right) + \left({}_{0}^{C} D_{t}^{\beta} \pi_{N}^{\frac{\beta}{2},0} \Phi_{1}^{k} - {}_{0}^{C} D_{t}^{\beta} \Phi_{1}^{k}, \upsilon_{N} \right) \\
= \left(\pi_{N}^{\frac{\alpha}{2},0} \left(D_{\tau}^{\beta} \Phi_{1}^{k} - {}_{0}^{C} D_{t}^{\alpha} \Phi_{1}^{k} \right), \upsilon_{N} \right) - \left({}_{0}^{C} D_{t}^{\beta} \tilde{e}_{1,N}^{k}, \upsilon_{N} \right) \\
\stackrel{\Delta}{=} \mathcal{E}_{31}^{k} + \mathcal{E}_{32}^{k},$$
(3.29)

by combining the results of (3.5), the Hölder inequality, and the Young inequality, we have

$$\begin{aligned} \mathcal{E}_{31}^{k} &\leq \frac{\epsilon_{1}}{2} \left\| \pi_{N}^{\frac{\alpha}{2},0} \left(D_{\tau}^{\beta} \Phi_{1}^{k} - {}_{0}^{C} D_{t}^{\beta} \Phi_{1}^{k} \right) \right\|^{2} + \frac{1}{2\epsilon_{1}} \left\| \upsilon_{N} \right\|^{2} \\ &\leq \frac{\epsilon_{1}}{2} C_{1} \left\| D_{\tau}^{\beta} \Phi_{1}^{k} - {}_{0}^{C} D_{t}^{\beta} \Phi_{1}^{k} \right\|^{2} + \frac{1}{2\epsilon_{1}} \left\| \upsilon_{N} \right\|^{2} \\ &\leq \frac{\epsilon_{1}}{2} C_{1,\Phi_{1}} \tau^{4-2\beta} + \frac{1}{2\epsilon_{1}} \left\| \upsilon_{N} \right\|^{2}, \end{aligned}$$

furthermore, by means of Lemma 0.2, we have

$$\mathcal{E}_{32}^{k} \leq \frac{\epsilon_{1}}{2} C_{1} N^{\alpha - 2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi_{1}^{k} \right\|_{s}^{2} + \frac{1}{2\epsilon_{1}} \left\| v_{N} \right\|^{2} \\ \leq \frac{\epsilon_{1}}{2} C_{1} N^{\alpha - 2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi_{1} \right\|_{s}^{2} + \frac{1}{2\epsilon_{1}} \left\| v_{N} \right\|^{2}.$$

Thus (3.29) becomes

$$\mathcal{E}_{3}^{k} \leq \frac{1}{\epsilon_{1}} \left\| v_{N} \right\|^{2} + \frac{\epsilon_{1}}{2} C_{1} N^{\alpha - 2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi_{1} \right\|_{s}^{2} + \frac{\epsilon_{1}}{2} C_{1, \Phi_{1}} \tau^{4 - 2\beta}.$$
(3.30)

For the fourth term \mathcal{E}_4^k , it holds by invoking Remark 0.2

$$\mathcal{E}_{4}^{k} \leq \frac{\epsilon_{1}}{2} C_{1} N^{\alpha - 2r} \left\| \Phi_{1} \right\|_{r}^{2} + \frac{1}{2\epsilon_{1}} \left\| \upsilon_{N} \right\|^{2}.$$
(3.31)

Substituting (3.27), (3.28), (3.30) and (3.31) into (3.22), we can infer that

$$(D_{\tau}^{\beta} \hat{e}_{1,N}^{k}, \upsilon_{N}) + A(\hat{e}_{1,N}^{k}, \upsilon_{N})$$

$$\leq \frac{3}{\epsilon_{1}} \|\upsilon_{N}\|^{2} + 4\epsilon_{1}C_{1}L_{1}^{2} \|\hat{e}_{1,N}^{k-1}\|^{2} + \epsilon_{1}C_{1}L_{1}^{2} \|\hat{e}_{1,N}^{k-2}\|^{2} + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \|\hat{e}_{1,N}^{k-N_{s}}\|^{2} + \tilde{\mathcal{K}}_{1},$$

$$(3.32)$$

where

$$\tilde{\mathcal{R}}_{1} = \frac{\epsilon_{1}}{2} \tilde{C}_{1} N^{\alpha - 2s} \left(\left\| {}_{0}^{C} D_{t}^{\beta} \Phi_{1} \right\|_{s}^{2} + \left\| \Phi_{1} \right\|_{s}^{2} \right) + \frac{\epsilon_{1}}{2} \tilde{C}_{1} N^{-2r} \left\| \Phi_{1} \right\|_{r}^{2} + \epsilon_{1} \tilde{C}_{1 \Phi_{1}} \left(\tau^{4} + \tau^{4 - 2\beta} \right),$$

such that $\tilde{C}_{1\Phi_1} := 2 \max\{C_{1,\Phi_1}, \tilde{c}_{\Phi_1}\}$. Taking $v_N = \hat{e}_{1,N}^k$ in (3.32) and applying (22), we can conclude that

$$\frac{1}{2}D_{\tau}^{\beta} \left\| \hat{e}_{1,N}^{k} \right\|^{2} + \left\| \hat{e}_{1,N}^{k} \right\|_{\alpha/2}^{2} \leq \frac{5}{2\epsilon_{1}} \left\| \hat{e}_{1,N}^{k} \right\|^{2} + 4\epsilon_{1}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-1} \right\|^{2} + \epsilon_{1}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-2} \right\|^{2} + \frac{\epsilon_{1}}{2}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-N_{s}} \right\|^{2} + \tilde{\mathcal{R}}_{1},$$

namely,

$$D_{\tau}^{\beta} \left\| \hat{e}_{1,N}^{k} \right\|^{2} \leq \frac{6}{\epsilon_{1}} \left\| \hat{e}_{1,N}^{k} \right\|^{2} + 8\epsilon_{1}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-1} \right\|^{2} + 2\epsilon_{1}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-2} \right\|^{2} + \epsilon_{1}C_{1}L_{1}^{2} \left\| \hat{e}_{1,N}^{k-N_{s}} \right\|^{2} + \mathcal{R}_{1},$$

$$(3.33)$$

with $\mathcal{R}_1 = 2\tilde{\mathcal{R}}_1$. The same steps can be used to arrive at the same conclusion for (3.15) and (3.21) at j = 2, i.e.,

$$D_{\tau}^{\beta} \left\| \hat{e}_{2,N}^{k} \right\|^{2} \leq \frac{6}{\epsilon_{2}} \left\| \hat{e}_{2,N}^{k} \right\|^{2} + 8\epsilon_{2}C_{2}L_{2}^{2} \left\| \hat{e}_{2,N}^{k-1} \right\|^{2} + 2\epsilon_{2}C_{2}L_{2}^{2} \left\| \hat{e}_{2,N}^{k-2} \right\|^{2} + \epsilon_{2}C_{2}L_{2}^{2} \left\| \hat{e}_{2,N}^{k-N_{s}} \right\|^{2} + \mathcal{R}_{2},$$

$$(3.34)$$

where

$$\mathcal{R}_{2} = 2\tilde{\mathcal{R}}_{2} = \frac{\epsilon_{2}}{2}\tilde{C}_{2}N^{\alpha-2s} \left(\left\| {}_{0}^{C}D_{t}^{\beta}\Phi_{2} \right\|_{s}^{2} + \left\| \Phi_{2} \right\|_{s}^{2} \right) + \frac{\epsilon_{2}}{2}\tilde{C}_{2}N^{-2r} \left\| \Phi_{2} \right\|_{r}^{2} + \epsilon_{2}\tilde{C}_{2}\Phi_{2} \left(\tau^{4} + \tau^{4-2\beta} \right).$$

Adding (3.33) and (3.34) together, we obtain

$$D_{\tau}^{\beta} \left(\left\| \hat{e}_{1,N}^{k} \right\|^{2} + \left\| \hat{e}_{2,N}^{k} \right\|^{2} \right)$$

$$\leq \frac{12}{\min\{\epsilon_{1},\epsilon_{2}\}} \left(\left\| e_{1,N}^{k} \right\|^{2} + \left\| e_{2,N}^{k} \right\|^{2} \right) + 16\hat{C} \left(\left\| e_{1,N}^{k-1} \right\|^{2} + \left\| e_{2,N}^{k-1} \right\|^{2} \right)$$

$$+ 4\hat{C} \left(\left\| e_{1,N}^{k-2} \right\|^{2} + \left\| e_{2,N}^{k-2} \right\|^{2} \right) + 2\hat{C} \left(\left\| e_{1,N}^{k-N_{s}} \right\|^{2} + \left\| e_{2,N}^{k-N_{s}} \right\|^{2} \right) + \hat{\mathcal{R}},$$

where $\hat{C} = \max\{\epsilon_1 C_1 L_1^2, \epsilon_2 C_2 L_2^2\}$ and $\hat{\mathcal{R}} = \max\{\mathcal{R}_1, \mathcal{R}_2\}$. By means of Lemma 0.11 and since $\min\{\epsilon_1, \epsilon_2\} > 0$, there exists a positive constant $\tau^* = \sqrt[\beta]{1/\left(2\Gamma(2-\beta)\frac{12}{\min\{\epsilon_1,\epsilon_2\}}\right)}$, when $\tau < \tau^*$, we have

$$\left\| \hat{e}_{1,N}^{k} \right\|^{2} + \left\| \hat{e}_{2,N}^{k} \right\|^{2} \leq \frac{2\hat{\mathcal{R}}t_{k}^{\beta}}{\Gamma(1+\beta)} E_{\beta}(2\mu t_{k}^{\beta}),$$

with $\mu = \frac{12}{\min\{\epsilon_1, \epsilon_2\}} + 16\hat{C}/(a_0 - a_1) + 4\hat{C}/(a_1 - a_2) + 2\hat{C}/(a_{N_s-1} - a_{N_s})$. As a result, the scheme is unconditionally convergent. Applying the triangle inequality and Lemma 0.2, the proof of (3.20) is then completed.

3.4 Numerical simulations

Here, we provide a numerical examples to explain better the suggested system's temporal and spatial convergence orders. Also, we investigate the new effects which obtained by introducing fractional delayed Schnackenberg model (3.3) in comparison with integer model (1). In order to investigate both temporal and spatial convergence orders independently, we'll calculate the orders of convergence in both of them using the L2-error norms (1.50).

Example 3.1. Consider the following diffusive Schnakenberg system with time delay s = 0.5:

$$\begin{aligned}
\frac{\partial^{\beta} \Phi_{1}(x,t)}{\partial t^{\beta}} &= \frac{\partial^{\alpha} \Phi_{1}(x,t)}{\partial |x|^{\alpha}} + 1 - \Phi_{1}(x,t) + \Phi_{2}(x,t-s) \left(1 + \Phi_{1}^{2}(x,t-s)\right) \\
&\quad + g_{1}(x,t), \quad x \in (0,1), \quad t > 0, \\
\frac{\partial^{\beta} \Phi_{2}(x,t)}{\partial t^{\beta}} &= \frac{\partial^{\alpha} \Phi_{2}(x,t)}{\partial |x|^{\alpha}} + 1 - \Phi_{2}(x,t-s) \left(1 + \Phi_{1}^{2}(x,t-s)\right) \\
&\quad + g_{2}(x,t), \quad x \in (0,1), \quad t > 0, \\
\Phi_{1}(0,t) &= \Phi_{2}(0,t) = \Phi_{1}(1,t) = \Phi_{2}(1,t) = 0, \quad t \ge 0, \\
\Phi_{1}(x,t) &= \frac{t^{4}}{\Gamma(5)}x^{2}(1-x)^{2} \ge 0, \quad (x,t) \in [0,1] \times [-s,0], \\
\Phi_{2}(x,t) &= \frac{t^{3}}{\Gamma(4)}x^{2}(1-x)^{2} \ge 0, \quad (x,t) \in [0,1] \times [-s,0].
\end{aligned}$$
(3.35)

The exact solution is as $\Phi_1(x,t) = \frac{t^4}{\Gamma(5)}x^2(1-x)^2$ and $\Phi_2(x,t) = \frac{t^3}{\Gamma(4)}x^2(1-x)^2$.

The proposed method solves this example with different values of N, M, α , and β . Tables 4-7 present the errors associated with temporal convergence orders. It can be demonstrated from Tables 4-7 that the convergence rates in the time direction are consistent with the expected theoretical order convergence rate.

	7		I I I		
$\tau(N=50)$	Error	Order	N(M = 1600)	Error	AO
1/100	1.3627×10^{-7}		5	8.166×10^{-6}	$N^{-7.279}$
1/200	4.579×10^{-8}	1.573	10	7.035×10^{-7}	$N^{-6.152}$
1/400	1.529×10^{-8}	1.582	20	4.283×10^{-8}	$N^{-5.663}$
1/800	5.121×10^{-9}	1.577	30	9.212×10^{-9}	$N^{-5.440}$

Table 4: The rate of convergence and the errors for Φ_1 versus N and τ with $\beta = 0.4$ and $\alpha = 1.4$ for example 3.1.

Table 5: The rate of convergence and the errors for Φ_2 versus N and τ with $\beta = 0.4$ and $\alpha = 1.4$ for example 3.1.

$\tau(N=50)$	Error	Order	N(M = 1600)	Error	AO
1/100	2.693×10^{-7}		5	3.445×10^{-5}	$N^{-6.384}$
1/200	8.996×10^{-8}	1.582	10	2.844×10^{-6}	$N^{-5.546}$
1/400	2.995×10^{-8}	1.586	20	1.724×10^{-7}	$N^{-5.198}$
1/800	1.039×10^{-8}	1.526	30	3.342×10^{-8}	$N^{-5.061}$

Table 6: The rate of convergence and the errors for Φ_1 versus N and τ with $\beta = 0.9$ and $\alpha = 1.8$ for example 3.1.

	7		1		
$\tau(N=50)$	Error	Order	N(M = 800)	Error	AO
1/100	2.708×10^{-6}		5	4.163×10^{-6}	$N^{-7.697}$
1/200	1.266×10^{-6}	1.096	10	1.076×10^{-6}	$N^{-5.968}$
1/400	5.914×10^{-7}	1.098	20	2.825×10^{-7}	$N^{-5.033}$
1/800	2.760×10^{-7}	1.099	30	2.757×10^{-7}	$N^{-4.440}$

Table 7: The rate of convergence and the errors for Φ_2 versus N and τ with $\beta = 0.9$ and $\alpha = 1.8$ for example 3.1.

$\tau(N=50)$	$\tau(N=50)$ Error		N(M = 800)	Error	AO
1/100	2.708×10^{-6}		5	1.824×10^{-5}	$N^{-6.779}$
1/200	1.266×10^{-6}	1.98	10	4.260×10^{-7}	$N^{-5.370}$
1/400	5.914×10^{-7}	1.099	20	6.524×10^{-7}	$N^{-4.754}$
1/800	2.760×10^{-7}	1.100	30	5.914×10^{-7}	$N^{-4.216}$

In the following example, we show the effect of time and space fractional orders on the behavior of the dynamics for the solutions of the nonlinear delay fractional Schnakenberg model (3.3) in comparison with integer model (1).

Example 3.2. Consider the following Schnakenberg system:

$$\frac{\partial^{\beta} \Phi_{1}(x,t)}{\partial t^{\beta}} = \frac{\partial^{\alpha} \Phi_{1}(x,t)}{\partial |x|^{\alpha}} - \Phi_{1}(x,t) + \Phi_{1}^{2}(x,t-s)\Phi_{2}(x,t-s), \quad x \in (0,1), \quad t > 0, \\
\frac{\partial^{\beta} \Phi_{2}(x,t)}{\partial t^{\beta}} = \frac{\partial^{\alpha} \Phi_{2}(x,t)}{\partial |x|^{\alpha}} - \Phi_{1}^{2}(x,t-s)\Phi_{2}(x,t-s), \quad x \in (0,1), \quad t > 0, \\
\Phi_{1}(0,t) = \Phi_{2}(0,t) = \Phi_{1}(1,t) = \Phi_{2}(1,t) = 0, \quad t \ge 0, \\
\Phi_{1}(x,t) = e^{-2(x-5)^{2}} \ge 0, \quad \Phi_{2}(x,t) = e^{-2(x+5)^{2}} \ge 0, \quad (x,t) \in [0,1] \times [-s,0]. \\
(3.36)$$

Figures 3.1 and 3.2 show the profile of the behavior of the dynamics of the numerical solution for different values of β , α and s. In the figure 3.1, the first row is presented at $\alpha = 1.2$ and $\beta = 0.2$. The second row is presented at $\alpha = 1.5$ and $\beta = 0.5$. The third row is presented at $\alpha = 1.9$ and $\beta = 0.9$. In the figure 3.2, the presented row is done at $\alpha = 2.0$ and $\beta = 1.0$ (integer case). The delay is taken in the first column at s = 0.5, in the second column is presented at s = 1.5, and in the third column is presented at s = 3.0.

We can observe from these figures that the evolution of the solution is pretty sharp on the first time steps depending on β . We also find that the fractional-order parameter α affects the shape of the solutions. This effect is almightly clear for the the functions Φ_1 and Φ_2 in figure 3.1 in comparison with figure 3.2.

This means that the shape of solution becomes more smoothly when the values of β and α is taken as integer order ($\beta = 1.0$ and $\alpha = 2.0$, see model (1), presented in the introduction) as shown in the figure 3.2. We can deduce that the behavior of autocatalyst and reactant acted by the functions Φ_1 and Φ_2 are described more better in case of fractional order rather than integer ones. Also, we can say that the fractional-order parameters can be used in physics to modify the shape of waves without changing the non-linearity and dispersion effects of the fractional nonlinear models.



Figure 3.1 — The evolution of Φ_1 and Φ_2 for different values of $\beta = 0.2; 0.5; 0.9$, $\alpha = 1.2; 1.5; 1.9$ and s = 0.5; 1.5; 3.0.



Figure 3.2 — The evolution of Φ_1 and Φ_2 for the values of $\beta = 1.0$, $\alpha = 2.0$ and s = 0.5; 1.5; 3.0.

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Chapter 4 High-order numerical algorithm for the nonlinear time-space fractional reaction-diffusion equations with delay

In this chapter, we develop and provide numerical solutions to the nonlinear fractional order time-space diffusion equations with the influence of fixed temporal delay. An effective high-order numerical scheme that mixes the so-called Alikhanov $L2 - 1_{\sigma}$ formula side by side with the power of the Galerkin method is presented. Specifically, the time-fractional component is estimated using the uniform $L2 - 1_{\sigma}$ difference formula, while the spatial fractional operator is approximated using the Legendre-Galerkin spectral approximation. In addition, Taylor's approximations are used to discretize the term of the nonlinear source function. It has been shown theoretically that the suggested scheme's numerical solution is unconditionally stable, with a second-order time-convergence and a space-convergent order of exponential rate. Furthermore, a suitable discrete fractional Grönwall inequality is then utilized to quantify error estimates for the derived solution. Finally, we provide a numerical experiment that closely matches the theoretical investigation to assess the efficacy of the suggested method.

4.1 Preliminary results and problem formulation

One of the main challenges of the considered work is represented by how to numerically approximate the time Caputo fractional derivative. Indeed, substantial effort has been expended in the scientific literature to develop efficient formulas for approximating the time fractional derivatives in the Caputo sense. In what follows, we mention some of these works that relate to our problem under consideration. The L1 formula (1.3) is considered one of the most extensive methods used for the solution of fractional differential equations that include Caputo derivatives [52; 68; 172–176]. In the case of a non-uniform mesh, the L1 approximation provides a decent approximation when the mesh is refined close to the point t_{n+1} [177]. Even though the non-uniform mesh performs better than the uniform one, the second-order approximation will not be generated at all mesh nodes. In order to get a close approximation to the Caputo fractional derivative of order β (0 < β < 1), Gao et al.[178] constructed a novel formulation called the L1-2 formula with $3-\beta$ convergence order in temporal direction at time $t_k (k \ge 2)$. This formula is produced by approximating the integrated function with three points using a piecewise quadratic interpolation approximation and it is properly defined as a modification of the L1 formula with some correction terms added. In [179; 180], the Caputo time-fractional derivative is discretized by applying a numerical formula with $3 - \beta$ order, known as, the L2 formula. This formula is generated with the use of piecewise quadratic interpolating polynomials. Through the development of a discrete energy analysis approach, a comprehensive theoretical examination of the stability and convergence of this method is performed for every $\beta \in (0, 1)$. Alikhanov [77] devised a new difference scheme called the $L2 - 1_{\sigma}$ formula based on a high-order approximation for the Caputo fractional derivatives with $3 - \beta$ convergence order in temporal direction at time $t = t_k + \sigma$ with $\sigma = 1 - \frac{\beta}{2}$. It was shown in [181; 182] that the $L2 - 1_{\sigma}$ formula may be extended and used to solve the multi-term, distributed, variable-order time-fractional diffusion equations.

On the basis of this formula, a number of recent studies have investigated and developed high-order techniques for time fractional models in the Caputo sense. An implicit technique for solving fractional diffusion equations with time delay is shown in [183], which combines the Alikhanov formula for time approximation with the central difference method for spatial discretization. A second-order numerical approach was suggested by Nandal and Pandey in [184] for solving a nonlinear fourth-order delayed distributed fractional subdiffusion problem. They estimated the time-fractional derivative with the Alikhanov formula as well as the spatial dimensions with the compact difference operator. Following up on the $L2 - 1_{\sigma}$ formula, a slew of new works have appeared (see, for example, [185–187]).

Without loss of generality, in this chapter, we numerically propose a highorder algorithm for solving the following time-delayed nonlinear fractional order reaction-diffusion equations:

$$\frac{\partial^{\beta}\Phi}{\partial t^{\beta}} = \kappa \frac{\partial^{\alpha}\Phi}{\partial |x|^{\alpha}} + f(\Phi(x,t),\Phi(x,t-s)) + g(x,t), \quad x \in \Omega, \quad t \in I,$$
(4.1)

initialized and constrained by the conditions

$$\begin{cases} \Phi(x,t) = \psi(x,t), & x \in \Omega, \quad t \in [-s,0], \\ \Phi(a,t) = \Phi(b,t) = 0, \quad t \in I. \end{cases}$$
(4.2)

In this case, time and space domains are represented by $I = [0, T] \subset \mathbb{R}$ and $\Omega = [a, b] \subset \mathbb{R}$, respectively. Additionally, $\beta \in (0, 1)$ represents the temporal order of fractional time in which the time-fractional derivative is interpreted according to Caputo, whereas $\alpha \in (1, 2)$ represents the fractional order of space. The positive constants κ , and s, denote the diffusion and temporal delay parameters, respectively.

4.2 Derivation of Numerical Scheme

Here, in this section, we will focus on developing a high-order numerical approximation for the problem (4.1)-(4.2) based on combining Alikhanov $L2 - 1_{\sigma}$ difference formula and the spectral method of Legendre-Galerkin in order to discretize the temporal and space–fractional derivatives, respectively. We begin with temporal discretization following that, we detail the suggested scheme's spatial discretization.

4.2.1 Temporal discretization

We choose a time step given by $\tau = \frac{s}{N_s}$, where N_s is a positive integer, in order to uniformly divide the temporal domain I. This defines a class of uniform partitions denote by $t_k = k\tau$, for each $-N_s \leq k \leq M$, where $M = \left\lceil \frac{T}{\tau} \right\rceil$. Denote $t_{k+\sigma} = (k+\sigma)\tau = \sigma t_{k+1} + (1-\sigma)t_k$, for $k = 0, 1, \ldots, M$. Take $\Phi^{k+\sigma} = \Phi^{k+\sigma}(\cdot) = \Phi(\cdot, t_{k+\sigma})$.

In order to provide a semi-discretized form of (4.1)-(4.2) at each specified time $t_{k+\sigma}$, we estimate the time-fractional component using the uniform $L2 - 1_{\sigma}$ difference formula (29), while the nonlinear source term is discretized using Taylor's approximations (30). As a consequence, we obtain the following discrete-time system

$${}_{0}D^{\beta}_{\tau}\Phi^{k+\sigma} = \kappa \frac{\partial^{\alpha}\Phi^{k+\sigma}}{\partial |x|^{\alpha}} + f\left((\sigma+1)\Phi^{k} - \sigma\Phi^{k-1}, \sigma\Phi^{k+1-N_{s}} + (1-\sigma)\Phi^{k-N_{s}}\right) + g^{k+\sigma}(x), \quad x \in \Omega.$$

$$(4.3)$$

We also take into account initial-boundary approximations as the following form

$$\begin{cases} \Phi_i^k = \psi(x_i, t_k), & -N_s \le k \le 0, \quad x \in \Omega, \\ \Phi_0^k = \Phi_M^k(x) = 0, & -N_s \le k \le 0, \quad x \in \Omega, \end{cases}$$
(4.4)

According to Lemmas 0.8 and 0.10, this semi-scheme is technically accurate to the second order. Later in this context, a comprehensive study of the convergence rate for the full-discrete scheme will be provided. Next, we introduce the following two parameters:

$$\lambda_k^{(\beta,\sigma)} := \left(\frac{\mathcal{D}_{k+1}^{(k,\beta,\sigma)}}{\tau^{\beta}\Gamma(2-\beta)}\right)^{-1}, \qquad \tilde{\mathcal{D}}_j^{(k,\beta,\sigma)} := \begin{cases} \frac{\zeta_k^{(\beta,\sigma)} \ \mathcal{D}_j^{(k,\beta,\sigma)}}{\tau^{\beta}\Gamma(2-\beta)}, & 0 \le j \le k-1, \\ \frac{\zeta_k^{(\beta,\sigma)} \ \mathcal{D}_k^{(k,\beta,\sigma)}}{\tau^{\beta}\Gamma(2-\beta)}, & j = k. \end{cases}$$

Then, this permits the recasting of the semi-scheme (4.3) into the equivalent form

$$\Phi^{k+1} - \kappa \sigma \lambda_k^{(\beta,\sigma)} \frac{\partial^{\alpha} \Phi^{k+1}}{\partial |x|^{\alpha}} = \kappa (1-\sigma) \lambda_k^{(\beta,\sigma)} \frac{\partial^{\alpha} \Phi^k}{\partial |x|^{\alpha}} - \sum_{j=0}^k \tilde{\mathcal{D}}_{j,l}^{(k,\beta,\sigma)} \Phi^j + \lambda_k^{(\beta,\sigma)} f\left((\sigma+1) \Phi^k - \sigma \Phi^{k-1}, \sigma \Phi^{k+1-N_s} + (1-\sigma) \Phi^{k-N_s}\right) + g^{k+1}.$$
(4.5)

4.2.2 Spatial discretization

We first present the space function below to give suitable base functions that precisely meet the boundary requirements specified in spectral techniques for space fractional order equations in order to linearize the space-fractional components [118; 133]:

$$\mathcal{W}_N^0 = \mathcal{P}_N(\Omega) \cap H_0^1(\Omega) = \operatorname{span} \left\{ \varphi_n(x) : n = 0, 1, \dots, N - 2 \right\},$$
(4.6)

where φ_n symbolizes the base functions, which are represented by the Legendre polynomial as:

$$\varphi_n(x) = L_n(\hat{x}) - L_{n+2}(\hat{x}) = \frac{2n+3}{2(n+1)}(1-\hat{x}^2) \ J_n^{1,1}(\hat{x}), \quad \forall \ \hat{x} \in [-1,1], \quad (4.7)$$

where $x = \frac{1}{2}((b-a)\hat{x} + a + b) \in [a, b]$. Therefore, the fully discrete $L2 - 1_{\sigma}$ Galerkin spectral scheme for (4.5) can be expressed as follows: find $\Phi^{k+1} \in \mathcal{W}_N^0$, $k \ge 0$ such that satisfying the following system:

$$\begin{cases} \left(\Phi^{k+1}, \upsilon\right) - \kappa \sigma \lambda_{k}^{(\beta,\sigma)} \left(\frac{\partial^{\alpha} \Phi^{k+1}}{\partial |x|^{\alpha}}, \upsilon\right) = \kappa (1-\sigma) \lambda_{k}^{(\beta,\sigma)} \left(\frac{\partial^{\alpha} \Phi^{k}}{\partial |x|^{\alpha}}, \upsilon\right) - \sum_{j=0}^{k} \tilde{\mathcal{D}}_{j,l}^{(k,\beta,\sigma)} \left(\Phi^{j}, \upsilon\right) \\ + \lambda_{k}^{(\beta,\sigma)} \left(I_{N} f\left((\sigma+1) \Phi^{k} - \sigma \Phi^{k-1}, \sigma \Phi^{k+1-N_{s}} + (1-\sigma) \Phi^{k-N_{s}}\right), \upsilon\right) \\ + \left(I_{N} g^{k+1}(x), \upsilon\right), \quad k \ge 0, \quad \forall \ \upsilon \in W_{N}^{0}, \\ \Phi_{N}^{0} = \pi_{N}^{1,0} \psi, \end{cases}$$

$$(4.8)$$

where $\pi_N^{1,0}$ is a suitable projection operator in this case. Following this, we could further generalize the approximation as

$$\Phi_N^{k+1} = \sum_{i=0}^{N-2} \hat{\Phi}_i^{k+1} \varphi_i(x), \qquad (4.9)$$

where $\hat{\Phi}_i^{k+1}$ are an undetermined expansion coefficients. The uniform full discrete scheme for (4.1)-(4.2) can be expressed as a linear system in a matrix form using (4.9), lemma 0.1 and allowing $v = \varphi_k$, for each $0 \le k \le N - 2$ as follows:

$$\left(\bar{M} - \kappa \sigma \lambda_k^{(\beta,\sigma)} (S + S^T)\right) U^{k+1} = R^k + \lambda_k^{(\beta,\sigma)} H^k + G^{k+1}, \qquad (4.10)$$

where the notations in the above expression are given by

$$\begin{split} s_{ij} &= \int_{\Omega} {}_{a} D_{x}^{\frac{\alpha}{2}} \varphi_{i}(x)_{x} D_{b}^{\frac{\alpha}{2}} \varphi_{j}(x) dx, \qquad S = (s_{ij})_{i,j=0}^{N-2}, \\ m_{ij} &= \int_{\Omega} \varphi_{i}(x) \varphi_{j}(x) dx, \qquad \bar{M} = (m_{ij})_{i,j=0}^{N-2}, \\ h_{i}^{k} &= \int_{\Omega} \varphi_{i}(x) I_{N} f\left((\sigma+1) \ \Phi^{k} - \sigma \ \Phi^{k-1}, \sigma \ \Phi^{k+1-N_{s}} + (1-\sigma) \ \Phi^{k-N_{s}}\right) dx, \\ H^{k} &= (h_{0}^{k}, h_{1}^{k}, \dots, h_{N-2}^{k})^{\top}, \qquad U^{k+1} = \left(\hat{\Phi}_{0}^{k+1}, \hat{\Phi}_{1}^{k+1}, \dots, \hat{\Phi}_{N-2}^{k+1}\right)^{\top}, \\ g_{i}^{k+1} &= \int_{\Omega} \varphi_{i}(x) I_{N} g^{k+1} dx, \qquad G^{k+1} = (g_{0}^{k+1}, g_{1}^{k+1}, \dots, g_{N-2}^{k+1})^{\top}, \\ R^{k} &= \kappa (1-\sigma) \lambda_{k}^{(\beta,\sigma)} (S+S^{T}) \Phi^{k} - \tilde{\mathcal{D}}_{l}^{(k,\beta,\sigma)} \bar{M} \Phi^{k}. \end{split}$$

The elements of the stiffness matrix S and the mass matrix \overline{M} can be easily calculated using lemma 1.1.

4.3 Theoretical analysis

This section aims to verify how effectively the numerical solution of the suggested approach for the problem (4.1)-(4.2). We start with stability analysis and give the theorem of stability in the first subsection. The second subsection is devoted to the convergence analysis and the theorem of convergence is given there. We assume that the Lipschitz condition below holds for the function f, which is necessary for the theoretical analysis, i.e,

$$|f(\Phi_1, v_1) - f(\Phi_2, v_2)| \le L \left(|\Phi_1 - \Phi_2| + |v_1 - v_2| \right), \tag{4.11}$$

where L is a positive constant.

4.3.1 Stability analysis

The variation formulation of the proposed scheme can be obtained by means of (14), (4.3) side by side with lemma 0.10. More specifically, need to find $\{\Phi_N^k\}_{k=1}^M \in \mathcal{P}_N$, such that satisfying the following:

$$\begin{pmatrix} D_{\tau}^{\beta} \Phi_{N}^{k+\sigma}, \upsilon_{N} \end{pmatrix} + A \left(\Phi_{N}^{k+\sigma}, \upsilon_{N} \right)$$

$$= \left(I_{N} f \left((\sigma+1) \Phi_{N}^{k} - \sigma \; \Phi_{N}^{k-1}, \sigma \; \Phi_{N}^{k+1-N_{s}} + (1-\sigma) \Phi_{N}^{k-N_{s}} \right), \upsilon \right)$$

$$+ \left(I_{N} g^{k+\sigma}, \upsilon \right), \quad \forall \upsilon_{N} \in \mathcal{P}_{N},$$

$$(4.12)$$

with initial conditions

$$\Phi_N^k = \pi_N^{1,0} \varphi^k, \ -N_s \le k \le 0.$$

Due to the linear iterative nature of the method, a solution to an algebraic equation system is all that is required at each iteration. The suggested scheme's well-posedness, meaning it is uniquely solvable and continues to rely on its initial boundary conditions which is sufficient to hold the Lax-Milgram lemma's assumptions. [136]. In particular, it can be seen from equation (4.12) that the bilinear shape $A(\cdot, \cdot)$ is continuous as well as coercive related to $H_0^{\alpha/2} \times H_0^{\alpha/2}$. We further presume that $\{\tilde{\Phi}_N^k\}_{k=1}^M$ is the solution of the following variational form

$$\begin{pmatrix}
D_{\tau}^{\beta}\tilde{\Phi}_{N}^{k+\sigma},\upsilon_{N}\end{pmatrix} + A\left(\tilde{\Phi}_{N}^{k+\sigma},\upsilon_{N}\right) \\
= \left(I_{N}f\left((\sigma+1)\tilde{\Phi}_{N}^{k} - \sigma\tilde{\Phi}_{N}^{k-1},\sigma\tilde{\Phi}_{N}^{k+1-N_{s}} + (1-\sigma)\tilde{\Phi}_{N}^{k-N_{s}}\right),\upsilon\right) \\
+ \left(I_{N}\tilde{g}^{k+\sigma},\upsilon_{N}\right), \quad \forall \upsilon_{N} \in \mathcal{P}_{N},$$
(4.13)

with initial conditions

$$\tilde{\Phi}_N^k = \pi_N^{1,0} \varphi^k, \quad -N_{\mathbf{s}} \le k \le 0.$$

Now, we are ready to offer the stability theorem in the context of the subsequent discussion. **Theorem 4.1.** The suggested method (4.12) in this sense, is said to be unconditionally stable, which means it holds the following for $\tau > 0$,

$$\left\|\Phi_{N}^{k+\sigma} - \tilde{\Phi}_{N}^{k+\sigma}\right\|^{2} \le C \max_{1 \le k \le M} \left\|g^{k+\sigma} - \tilde{g}^{k+\sigma}\right\|^{2},$$

where C is a positive constant independent of N and τ .

Proof. Take $\rho_N^k = \Phi_N^k - \tilde{\Phi}_N^k$. Subtracting (4.13) from (4.12), then the error equation holds

$$(D_{\tau}^{\beta} \rho_{N}^{k+\sigma}, \upsilon_{N}) + A (\rho_{N}^{k+\sigma}, \upsilon_{N})$$

$$= (I_{N} f ((\sigma+1) \Phi_{N}^{k} - \sigma \Phi_{N}^{k-1}, \sigma \Phi_{N}^{k+1-N_{s}} + (1-\sigma) \Phi^{k-N_{s}})$$

$$-I_{N} f ((\sigma+1) \tilde{\Phi}_{N}^{k} - \sigma \tilde{\Phi}_{N}^{k-1}, \sigma \tilde{\Phi}_{N}^{k+1-N_{s}} + (1-\sigma) \tilde{\Phi}_{N}^{k-N_{s}}), \upsilon_{N})$$

$$+ (I_{N} g^{k+\sigma} - I_{N} \tilde{g}^{k+\sigma}, \upsilon_{N}).$$

$$(4.14)$$

Applying the Lipschitz condition (4.11) and using Hölder inequality side by side to Young inequality, we derive the following for the first term of the right-hand side

$$\begin{split} & \left(I_N f \left((\sigma+1) \Phi_N^k - \sigma \Phi_N^{k-1}, \sigma \Phi_N^{k+1-N_s} + (1-\sigma) \Phi^{k-N_s} \right) \right. \\ & \left. - I_N f \left((\sigma+1) \tilde{\Phi}_N^k - \sigma \tilde{\Phi}_N^{k-1}, \sigma \tilde{\Phi}_N^{k+1-N_s} + (1-\sigma) \tilde{\Phi}_N^{k-N_s} \right), \upsilon_N \right) \\ & \leq CL \left(\left\| (\sigma+1) \rho_N^k - \sigma \rho_N^{k-1} \right\| + \left\| \sigma \rho_N^{k+1-N_s} - (1-\sigma) \rho_N^{k-N_s} \right\| \right) \|\upsilon_N\| \\ & \leq \epsilon CL^2 \left\| (\sigma+1) \rho_N^k - \sigma \rho_N^{k-1} \right\|^2 + \epsilon CL^2 \left\| \sigma \rho_N^{k+1-N_s} - (1-\sigma) \rho_N^{k-N_s} \right\|^2 + \frac{1}{2\epsilon} \left\| \upsilon_N \right\|^2 \\ & \leq 2\epsilon CL^2 (\sigma+1)^2 \left\| \rho_N^k \right\|^2 + 2\epsilon CL^2 \sigma^2 \left\| \rho_N^{k-1} \right\|^2 + 2\epsilon CL^2 \sigma^2 \left\| \rho_N^{k+1-N_s} \right\|^2 \\ & \left. + 2\epsilon CL^2 (1-\sigma)^2 \left\| \rho_N^{k-N_s} \right\|^2 + \frac{1}{2\epsilon} \left\| \upsilon_N \right\|^2. \end{split}$$

Using the Hölder inequality, the Young inequality, as well as the interpolation operator property, we obtain the following for the second term

$$(I_N g^{k+\sigma} - I_N \tilde{g}^{k+\sigma}, v_N) \le \frac{\epsilon}{2} C \|g^{k+\sigma} - \tilde{g}^{k+\sigma}\|^2 + \frac{1}{2\epsilon} \|v_N\|^2.$$

Hence, (4.14) becomes

$$\begin{aligned} & \left(D_{\tau}^{\beta} \rho_{N}^{k+\sigma}, \upsilon_{N} \right) + A(\rho_{N}^{k+\sigma}, \upsilon_{N}) \\ & \leq \frac{1}{\epsilon} \left\| \upsilon_{N} \right\|^{2} + 2\epsilon C L^{2} (\sigma+1)^{2} \left\| \rho_{N}^{k} \right\|^{2} + 2\epsilon C L^{2} \sigma^{2} \left\| \rho_{N}^{k-1} \right\|^{2} + 2\epsilon C L^{2} \sigma^{2} \left\| \rho_{N}^{k+1-N_{s}} \right\|^{2} \\ & + 2\epsilon C L^{2} (1-\sigma) \left\| \rho_{N}^{k-N_{s}} \right\|^{2} + \frac{\epsilon}{2} C \left\| g^{k+\sigma} - \tilde{g}^{k+\sigma} \right\|^{2}. \end{aligned}$$

Taking $v_N = \rho_N^{k+\sigma}$ and using lemma 0.9 and (16), we deduce that

$$\begin{split} &\frac{1}{2}D_{\tau}^{\beta} \left\| \rho_{N}^{k+\sigma} \right\|^{2} + \left| \rho^{k+\sigma} \right|_{\alpha/2}^{2} \\ &\leq \frac{1}{\epsilon} \left\| \rho_{N}^{k+\sigma} \right\|^{2} + 2\epsilon CL^{2}(\sigma+1)^{2} \left\| \rho_{N}^{k} \right\|^{2} + 2\epsilon CL^{2}\sigma^{2} \left\| \rho_{N}^{k-1} \right\|^{2} + 2\epsilon CL^{2}\sigma^{2} \left\| \rho_{N}^{k+1-N_{s}} \right\|^{2} \\ &+ 2\epsilon CL^{2}(1-\sigma) \left\| \rho_{N}^{k-N_{s}} \right\|^{2} + \frac{\epsilon}{2}C \left\| g^{k+\sigma} - \tilde{g}^{k+\sigma} \right\|^{2}, \end{split}$$

following the omission of the second term in the left hand side, we have

$$\begin{split} &D_{\tau}^{\beta} \left\| \rho_{N}^{k+\sigma} \right\|^{2} \\ &\leq \frac{2}{\epsilon} \left\| \rho_{N}^{k+\sigma} \right\|^{2} + 4\epsilon CL^{2}(\sigma+1)^{2} \left\| \rho_{N}^{k} \right\|^{2} + 4\epsilon CL^{2}\sigma^{2} \left\| \rho_{N}^{k-1} \right\|^{2} + 4\epsilon CL^{2}\sigma^{2} \left\| \rho_{N}^{k+1-N_{s}} \right\|^{2} \\ &\quad + 4\epsilon CL^{2}(1-\sigma) \left\| \rho_{N}^{k-N_{s}} \right\|^{2} + \epsilon C \left\| g^{k+\sigma} - \tilde{g}^{k+\sigma} \right\|^{2} \\ &\leq \frac{4}{\epsilon} (\sigma+1)^{2} (1+C\epsilon^{2}L^{2}) \left\| \rho_{N}^{k} \right\|^{2} + \frac{4}{\epsilon} \sigma^{2} (1+C\epsilon^{2}L^{2}) \left\| \rho_{N}^{k-1} \right\|^{2} + 4\epsilon CL^{2}\sigma^{2} \left\| \rho_{N}^{k+1-N_{s}} \right\|^{2} \\ &\quad + 4\epsilon CL^{2} (1-\sigma)^{2} \left\| \rho_{N}^{k-N_{s}} \right\|^{2} + \epsilon C \left\| g^{k+\sigma} - \tilde{g}^{k+\sigma} \right\|^{2}. \end{split}$$

A direct application of Lemma 0.12, we find that for $\epsilon > 0$, there is some positive independent constant $\tau^* = \sqrt[\beta]{1/(2\Gamma(2-\beta) \frac{4}{\epsilon}(\sigma+1)^2(1+C\epsilon^2L^2))}$, such that when $\tau < \tau^*$, the following is hold.

$$\left\|\rho_{N}^{k+\sigma}\right\|^{2} \leq \frac{2\epsilon C t_{k}^{\beta}}{\Gamma(1+\beta)} E_{\beta}(2\mu t_{k}^{\beta}) \max_{1 \leq k \leq M} \left\|g^{k} - \tilde{g}^{k}\right\|^{2},$$

with

$$\mu = \frac{4}{\epsilon}(\sigma+1)^2(3+C\epsilon^2L^2) + \frac{4}{\epsilon}\frac{\sigma^2(3+C\epsilon^2L^2)}{b_0^{(\beta,\sigma)} - b_1^{(\beta,\sigma)}} + \frac{4\epsilon CL^2\sigma^2}{b_{N_s-2}^{(\beta,\sigma)} - b_{N_s-1}^{(\beta,\sigma)}} + \frac{4\epsilon CL^2(1-\sigma)^2}{b_{N_s-1}^{(\beta,\sigma)} - b_{N_s}^{(\beta,\sigma)}}.$$

4.3.2 Convergence

Here, we present the proof of the convergence theorem for the suggested scheme (4.12) using discrete error estimates.

Theorem 4.2. Let $\{\Phi^k\}_{k=-N_s}^M$ and $\{\Phi_N^k\}_{k=-N_s}^M$, be the exact and the approximate solutions for problem (4.1) and the proposed method (4.12), respectively. Assume that $\Phi \in C^2([0,T]; L^2(\Omega)) \cap C^1([0,T]; H^s(\Omega))$. Then for a positive constant Cindependent of N and τ , the following statement is valid

$$\left|\Phi^{k+\sigma} - \Phi^{k+\sigma}_N\right|_{\alpha/2} \le C\left(\tau^2 + N^{-r}\right), \quad 1 \le k \le M,\tag{4.15}$$

where r denotes the regularity order of the source term.

Proof. Take $\Phi^k - \Phi^k_N = e^k_N = (\Phi^k - \pi^{\frac{\alpha}{2},0}_N \Phi^k) + (\pi^{\frac{\alpha}{2},0}_N \Phi^k - \Phi^k_N) \stackrel{\Delta}{=} \tilde{e}^k_N + \hat{e}^k_N$. In addition, (4.1) has the following weak formulation:

$$\begin{pmatrix} {}^{C}_{0}D^{\beta}_{t}\Phi^{k+\sigma}, \upsilon_{N} \end{pmatrix} + A\left(\Phi^{k+\sigma}, \upsilon_{N}\right) = \left(f\left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_{s}}\right), \upsilon_{N}\right) + \left(g^{k+\sigma}, \upsilon_{N}\right).$$

$$(4.16)$$

By subtracting (4.12) from (4.16), and using the notion of orthogonal projection, then the error equation satisfy

$$(D^{\beta}_{\tau} \ \hat{e}^{k+\sigma}_N, \upsilon_N) + A(\hat{e}^{k+\sigma}_N, \upsilon_N) \stackrel{\Delta}{=} \mathcal{E}^{(k,\sigma)}_1 + \mathcal{E}^{(k,\sigma)}_2 + \mathcal{E}^{(k,\sigma)}_3 + \mathcal{E}^{(k,\sigma)}_4, \tag{4.17}$$

where

$$\begin{split} \mathcal{E}_{1}^{(k,\sigma)} &= \left(I_{N}f\left(\Phi^{k+\sigma}, \, \Phi^{k+\sigma-N_{s}}\right) \right. \\ &- I_{N}f\left((\sigma+1)\Phi_{N}^{k} - \sigma\Phi_{N}^{k-1}, \, \sigma\Phi_{N}^{k+1-N_{s}} + (1-\sigma)\Phi_{N}^{k-N_{s}}\right), \, \upsilon_{N} \right), \\ \mathcal{E}_{2}^{(k,\sigma)} &= \left(f\left(\Phi^{k+\sigma}, \, \Phi^{k+\sigma-N_{s}}\right) - I_{N}f\left(\Phi^{k+\sigma}, \, \Phi^{k+\sigma-N_{s}}\right), \, \upsilon_{N} \right), \\ \mathcal{E}_{3}^{(k,\sigma)} &= \left(D_{\tau}^{\beta} \, \pi_{N}^{\frac{\alpha}{2},0} \Phi^{k+\sigma} - {}_{0}^{C} \, D_{t}^{\beta} \Phi^{k+\sigma}, \, \upsilon_{N} \right), \\ \mathcal{E}_{4}^{(k,\sigma)} &= \left(g^{k+\sigma} - I_{N}g^{k+\sigma}, \, \upsilon_{N} \right). \end{split}$$

To proceed, we make an estimate of the terms $\mathcal{E}_1^{(k,\sigma)}$, $\mathcal{E}_2^{(k,\sigma)}$, $\mathcal{E}_3^{(k,\sigma)}$ and $\mathcal{E}_4^{(k,\sigma)}$ on the right-hand side. Regarding the first term $\mathcal{E}_1^{(k,\sigma)}$, we have

$$\begin{pmatrix}
I_N f \left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_s} \right) - I_N f \left((\sigma+1) \Phi^k - \sigma \Phi^{k-1}, \sigma \Phi^{k+1-N_s} + (1-\sigma) \Phi^{k-N_s} \right), \nu_N \\
+ \left(I_N f \left((\sigma+1) \Phi^k - \sigma \Phi^{k-1}, \sigma \Phi^{k+1-N_s} + (1-\sigma) \Phi^{k-N_s} \right) \\
- I_N f \left((\sigma+1) \Phi^k_N - \sigma \Phi^{k-1}_N, \sigma \Phi^{k+1-N_s}_N + (1-\sigma) \Phi^{k-N_s}_N \right), \nu_N \end{pmatrix} \\
\stackrel{\Delta}{=} \mathcal{E}_{11}^{(k,\sigma)} + \mathcal{E}_{12}^{(k,\sigma)}.$$
(4.18)

Invoking Taylor expansion holds

$$f\left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_s}\right) = f\left((\sigma+1)\Phi^k - \sigma\Phi^{k-1}, \sigma\Phi^{k+1-N_s} + (1+\sigma)\Phi^{k-N_s}\right) + \tilde{c}_{\Phi}\tau^2.$$

In addition, we use Hölder's and Young's inequalities to obtain

$$\mathcal{E}_{11}^{(k,\sigma)} \leq \left\| I_N f\left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_s}\right) - I_N f\left((\sigma+1)\Phi^k - \sigma\Phi^{k-1}, \sigma\Phi^{k+1-N_s} + (1-\sigma)\Phi^{k-N_s}\right) \right\| \|v_N\| \\ \leq C \left\| f\left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_s}\right) - f\left((\sigma+1)\Phi^k - \sigma\Phi^{k-1}, \sigma\Phi^{k+1-N_s} + (1-\sigma)\Phi^{k-N_s}\right) \right\| \|v_N\| \\ \leq \frac{\epsilon}{2} C \tilde{c}_{\Phi} \tau^4 + \frac{1}{2\epsilon} \|v_N\|^2.$$
(4.19)

By plugging into the Lipschitz condition (4.11) and using Hölder inequality side by side to Young inequality, we deduce that

$$\begin{aligned} \mathcal{E}_{12}^{(k,\sigma)} &\leq LC \left(\left\| (\sigma+1)e_{N}^{k} - \sigma e_{N}^{k-1} \right\| + \left\| \sigma e_{N}^{k+1-N_{s}} + (1-\sigma)e_{N}^{k-N_{s}} \right\| \right) \|v_{N}\| \\ &\leq \frac{\epsilon}{2}CL^{2} \left(\left\| (\sigma+1)\hat{e}_{N}^{k} - \sigma \hat{e}_{N}^{k-1} \right\| + \left\| \sigma \hat{e}_{N}^{k+1-N_{s}} + (1-\sigma)\hat{e}_{N}^{k-N_{s}} \right\| \right) \\ &+ \left\| (\sigma+1)\tilde{e}_{N}^{k} - \sigma \tilde{e}_{N}^{k-1} \right\| + \left\| \sigma \tilde{e}_{N}^{k+1-N_{s}} - (1-\sigma)\tilde{e}_{N}^{k-N_{s}} \right\| \right)^{2} + \frac{1}{2\epsilon} \|v_{N}\|^{2} \\ &\leq 2\epsilon CL^{2}(\sigma+1)^{2} \left\| \hat{e}_{N}^{k} \right\|^{2} + 2\epsilon CL^{2}\sigma^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + 2\epsilon CL^{2}\sigma^{2} \left\| \hat{e}_{N}^{k+1-N_{s}} \right\|^{2} \\ &+ 2\epsilon CL^{2}(1-\sigma)^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\|^{2} + 2\epsilon CL^{2}(\sigma+1)^{2} \left\| \tilde{e}_{N}^{k} \right\|^{2} + 2\epsilon CL^{2}\sigma^{2} \left\| \tilde{e}_{N}^{k-1} \right\|^{2} \\ &+ 2\epsilon CL^{2}\sigma^{2} \left\| \tilde{e}_{N}^{k+1-N_{s}} \right\|^{2} + 2\epsilon CL^{2}(1-\sigma)^{2} \left\| \tilde{e}_{N}^{k-N_{s}} \right\|^{2} + \frac{1}{2\epsilon} \left\| v_{N} \right\|^{2}. \end{aligned}$$
(4.20)

In addition, considering the Lemmas 0.2 and 0.3, it can be shown that

$$\left\| \tilde{e}_{N}^{k} \right\|^{2} \leq \frac{C}{C_{1}} N^{\alpha - 2s} \left\| \Phi^{k} \right\|_{s}^{2}, \qquad \left\| \tilde{e}_{N}^{k-1} \right\|^{2} \leq \frac{C}{C_{1}} N^{\alpha - 2s} \left\| \Phi^{k-1} \right\|_{s}^{2}, \\ \left\| \tilde{e}_{N}^{k+1-N_{s}} \right\|^{2} \leq \frac{C}{C_{1}} N^{\alpha - 2s} \left\| \Phi^{k+1-N_{s}} \right\|_{s}^{2}, \qquad \left\| \tilde{e}_{N}^{k-N_{s}} \right\|^{2} \leq \frac{C}{C_{1}} N^{\alpha - 2s} \left\| \Phi^{k-N_{s}} \right\|^{2},$$

then (4.20) becomes

$$\mathcal{E}_{12}^{(k,\sigma)} \leq 2\epsilon C L^2 (\sigma+1)^2 \left\| \hat{e}_N^k \right\|^2 + 2\epsilon C L^2 \sigma^2 \left\| \hat{e}_N^{k-1} \right\|^2 + 2\epsilon C L^2 \sigma^2 \left\| \hat{e}_N^{k+1-N_s} \right\|^2 + 2\epsilon C L^2 (1-\sigma)^2 \left\| \hat{e}_N^{k-N_s} \right\|^2 + \tilde{C} N^{\alpha-2s} \left\| \Phi \right\|_s^2 + \frac{1}{2\epsilon} \left\| v_N \right\|^2.$$
(4.21)

Substituting (4.19) and (4.21) into (4.18), we obtain that

$$\mathcal{E}_{1}^{(k,\sigma)} \leq \frac{1}{\epsilon} \|v_{N}\|^{2} + 2\epsilon CL^{2}(\sigma+1)^{2} \|\hat{e}_{N}^{k}\|^{2} + 2\epsilon CL^{2}\sigma^{2} \|\hat{e}_{N}^{k-1}\|^{2} + 2\epsilon CL^{2}\sigma^{2} \|\hat{e}_{N}^{k+1-N_{s}}\|^{2} + 2\epsilon CL^{2}(1-\sigma)^{2} \|\hat{e}_{N}^{k-N_{s}}\|^{2} + \tilde{C}N^{\alpha-2s} \|\Phi\|_{s}^{2} + \frac{\epsilon}{2}\tilde{c}_{\Phi}\tau^{4}.$$
(4.22)

Hölder's inequality, Young's inequality, and Lemma 0.5 allow us to deduce the following for the second term $\rho_2^{(k,\sigma)}$ as follows

$$\mathcal{E}_{2}^{(k,\sigma)} \leq \left\| f\left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_{s}}\right) - I_{N}f\left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_{s}}\right) \right\| \|\upsilon_{N}\|$$

$$\leq \frac{\epsilon}{2} \left\| f\left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_{s}}\right) - I_{N}f\left(\Phi^{k+\sigma}, \Phi^{k+\sigma-N_{s}}\right) \right\|^{2} + \frac{1}{2\epsilon} \left\|\upsilon_{N}\right\|^{2}$$

$$\leq \frac{1}{2\epsilon} \left\|\upsilon_{N}\right\|^{2} + \frac{\epsilon}{2}CN^{-2r} \left\|\Phi\right\|_{s}^{2}.$$
(4.23)

For the third term \mathcal{E}_3^k , it holds

$$\mathcal{E}_{3}^{(k,\sigma)} = \left(D_{\tau}^{\beta} \pi_{N}^{\frac{\alpha}{2},0} \Phi^{k+\sigma} - {}_{0}^{C} D_{t}^{\beta} \pi_{N}^{\frac{\alpha}{2},0} \Phi^{k+\sigma}, \upsilon_{N} \right) + \left({}_{0}^{C} D_{t}^{\beta} \pi_{N}^{\frac{\beta}{2},0} \Phi^{k+\sigma} - {}_{0}^{C} D_{t}^{\beta} \Phi^{k+\sigma}, \upsilon_{N} \right) \\
= \left(\pi_{N}^{\frac{\alpha}{2},0} \left(D_{\tau}^{\beta} \Phi^{k+\sigma} - {}_{0}^{C} D_{t}^{\alpha} \Phi^{k+\sigma} \right), \upsilon_{N} \right) - \left({}_{0}^{C} D_{t}^{\beta} \tilde{e}_{N}^{k+\sigma}, \upsilon_{N} \right) \\
\stackrel{\Delta}{=} \mathcal{E}_{31}^{(k,\sigma)} + \mathcal{E}_{32}^{(k,\sigma)}, \qquad (4.24)$$

combining (26) with Hölder inequality and Young inequality yields

$$\begin{aligned} \mathcal{E}_{31}^{(k,\sigma)} &\leq \frac{\epsilon}{2} \left\| \pi_{N}^{\frac{\alpha}{2},0} \left(D_{\tau}^{\beta} \Phi^{k+\sigma} - {}_{0}^{C} D_{t}^{\beta} \Phi^{k+\sigma} \right) \right\|^{2} + \frac{1}{2\epsilon} \| v_{N} \|^{2} \\ &\leq \frac{\epsilon}{2} C \left\| D_{\tau}^{\beta} \Phi^{k+\sigma} - {}_{0}^{C} D_{t}^{\beta} \Phi^{k+\sigma} \right\|^{2} + \frac{1}{2\epsilon} \| v_{N} \|^{2} \\ &\leq \frac{\epsilon}{2} C \Phi \tau^{9-2\beta} + \frac{1}{2\epsilon} \| v_{N} \|^{2}, \end{aligned}$$

furthermore, by means of Lemma 0.2, we have

$$\mathcal{E}_{32}^{(k,\sigma)} \leq \frac{\epsilon}{2} C N^{\alpha-2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi^{k+\sigma} \right\|_{s}^{2} + \frac{1}{2} \left\| v_{N} \right\|^{2} \\ \leq \frac{\epsilon}{2} C N^{\alpha-2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi \right\|_{s}^{2} + \frac{1}{2\epsilon} \left\| v_{N} \right\|^{2}.$$

Thus (4.24) becomes

$$\mathcal{E}_{3}^{(k,\sigma)} \leq \frac{1}{\epsilon} \left\| \upsilon_{N} \right\|^{2} + \frac{\epsilon}{2} C N^{\alpha-2s} \left\| {}_{0}^{C} D_{t}^{\beta} \Phi \right\|_{s}^{2} + \frac{\epsilon}{2} C_{\Phi} \tau^{9-2\beta}.$$

$$(4.25)$$

By the aid of Remark 0.2, we obtain the following for the fourth term $\mathcal{E}_4^{(k,\sigma)}$

$$\mathcal{E}_{4}^{(k,\sigma)} \leq \frac{\epsilon}{2} C N^{\alpha-2r} \|\Phi\|_{r}^{2} + \frac{1}{2\epsilon} \|\upsilon_{N}\|^{2}.$$
(4.26)

Substituting (4.22), (4.23), (4.25) and (4.26) into (4.17), we can infer that

where

$$\tilde{\mathcal{R}} = \epsilon \tilde{C} N^{\alpha - 2s} \left(\left\| \Phi \right\|_s^2 + \left\|_0^C D_t^\beta \Phi \right\|_s^2 \right) + \epsilon \tilde{C} N^{-2r} \left\| \Phi \right\|_r^2 + \epsilon \tilde{C}_\Phi \left(\tau^4 + \tau^{9 - 2\beta} \right)$$

Taking $v_N = \hat{e}_N^{k+\sigma}$ in (4.27) and applying Lemma 0.9, we can conclude that

$$\begin{split} &\frac{1}{2}D_{\tau}^{\beta} \left\| \hat{e}_{N}^{k+\sigma} \right\|^{2} + |\hat{e}_{N}^{k+\sigma}|_{\alpha/2}^{2} \\ &\leq \frac{3}{\epsilon} \left\| \hat{e}_{N}^{k+\sigma} \right\|^{2} + 2\epsilon CL^{2}(\sigma+1)^{2} \left\| \hat{e}_{N}^{k} \right\|^{2} + 2\epsilon CL^{2}\sigma^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + 2\epsilon CL^{2}\sigma^{2} \left\| \hat{e}_{N}^{k+1-N_{s}} \right\|^{2} \\ &+ 2\epsilon CL^{2}(1-\sigma)^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\| + \tilde{\mathcal{R}}, \end{split}$$

hence, after omitting the second term on the left side of the above equation, we get

$$D_{\tau}^{\beta} \left\| \hat{e}_{N}^{k} \right\|^{2} \leq \frac{6}{\epsilon} \left\| \hat{e}_{N}^{k+\sigma} \right\|^{2} + 4\epsilon CL^{2}(\sigma+1)^{2} \left\| \hat{e}_{N}^{k} \right\|^{2} + 4\epsilon CL^{2}\sigma^{2} \left\| \hat{e}_{N}^{k-1} \right\|^{2} + 4\epsilon CL^{2}\sigma^{2} \left\| \hat{e}_{N}^{k+1-N_{s}} \right\|^{2} + 4\epsilon CL^{2}(1-\sigma)^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\| + \mathcal{R} \leq \frac{4}{\epsilon} (\sigma+1)^{2} (3+C\epsilon^{2}L^{2}) \left\| \hat{e}^{k} \right\|^{2} + \frac{4}{\epsilon} \sigma^{2} (3+C\epsilon^{2}L^{2}) \left\| \hat{e}^{k-1} \right\|^{2} + 4\epsilon CL^{2}\sigma^{2} \left\| \hat{e}_{N}^{k+1-N_{s}} \right\|^{2} + 4\epsilon CL^{2} (1-\sigma)^{2} \left\| \hat{e}_{N}^{k-N_{s}} \right\| + \mathcal{R},$$

with $\mathcal{R} = 2\tilde{\mathcal{R}}$. By means of Lemma 0.12 we find that for $\epsilon > 0$, there is some positive independent constant $\tau^* = \sqrt[\beta]{1/(2\Gamma(2-\beta)\frac{4}{\epsilon}(\sigma+1)^2(3+C\epsilon^2L^2))}$, when $\tau < \tau^*$, we have

$$\left\|e_N^{k+\sigma}\right\|^2 \le \frac{2\mathcal{R}Ct_k^\beta}{\Gamma(1+\beta)}E_\beta(2\mu t_k^\beta),$$

with

$$\mu = \frac{6}{\epsilon} + \frac{2\epsilon CL^2(\sigma+1)^2}{b_0^{(\beta,\sigma)} - b_1^{(\beta,\sigma)}} + \frac{2\epsilon CL^2\sigma^2}{b_1^{(\beta,\sigma)} - b_2^{(\beta,\sigma)}} + \frac{2\epsilon CL^2\sigma^2}{b_{N_s-2}^{(\beta,\sigma)} - b_{N_s-1}^{(\beta,\sigma)}} + \frac{2\epsilon CL^2(1-\sigma)}{b_{N_s-1}^{(\beta,\sigma)} - b_{N_s}^{(\beta,\sigma)}} + \frac{2\epsilon CL^2(1-\sigma)}{b_{N_s-1}^{(\beta,\sigma)} - b_{N_s}^{(\beta,\sigma)} - b_{N_s}^{(\beta,\sigma)}} + \frac{2\epsilon CL^2(1-\sigma)}{b_{N_s-1}^{(\beta,\sigma)} - b_{N_s}^{(\beta,\sigma)} - b_{N_s$$

Consequently, the scheme converges regardless of circumstances. The triangle inequality and (18) were then combined to complete the (4.15) proof.

4.4 Numerical simulations

As such, we perform a test example to further characterize the suggested system's temporal and spatial convergence orders. We also show how the dynamics of the solution to systems of fractional diffusion equations with delay are affected by fractional orders in the temporal and spatial directions. In order to investigate both temporal and spatial convergence orders independently, we'll calculate the orders of convergence in both of them using the L2-error norms (1.50).

Example 4.1. Consider the following nonlinear delayed diffusion problem

$$\frac{\partial^{\beta}\Phi}{\partial t^{\beta}}(x,t) = \frac{\partial^{\alpha}\Phi}{\partial |x|^{\alpha}}(x,t) - 2\Phi(x,t) + \frac{\Phi(x,t-0.1)}{1+\Phi^{2}(x,t-0.1)} + g(x,t), \ x \in (0,1), \ t \in (0,1],$$
(4.28)

such that problem (4.28) admits an exact solution $\frac{t^2}{\Gamma(3)}x^2(1-x)^2$ with respect to a given function g(x,t).

				1			
	au	$\alpha - 1 = \beta = 0.1$		$\alpha - 1 = \beta = 0.5$		$\alpha - 1 = \beta = 0.9$	
	1	Error	Order	Error	Order	Error	Order
	0.1/5	2.612×10^{-7}		4.076×10^{-6}		2.449×10^{-5}	
L1	0.1/10	7.466×10^{-8}	1.807	1.454×10^{-6}	1.487	1.143×10^{-5}	1.099
	0.1/15	3.588×10^{-8}	1.807	7.943×10^{-7}	1.491	7.319×10^{-6}	1.100
	0.1/20	2.156×10^{-8}	1.771	5.168×10^{-7}	1.494	5.334×10^{-6}	1.100
	0.1/25	1.481×10^{-8}	1.682	3.702×10^{-7}	1.495	4.173×10^{-6}	1.100
$L2 - 1_{\sigma}$	0.1/5	2.341×10^{-7}		1.030×10^{-6}		1.909×10^{-6}	
	0.1/10	5.893×10^{-8}	1.990	2.572×10^{-7}	2.001	4.773×10^{-7}	1.999
	0.1/15	2.622×10^{-8}	1.997	1.143×10^{-7}	2.000	2.122×10^{-7}	1.999
	0.1/20	1.473×10^{-8}	2.004	6.435×10^{-8}	1.997	1.194×10^{-7}	1.997
	0.1/25	9.405×10^{-9}	2.010	4.123×10^{-8}	1.995	7.652×10^{-8}	1.995

Table 8: The rate of convergence and the associate errors for Φ versus N and τ with N = 100 for example 4.1

As shown in table 8, a comparison between the L2-errors and their accompanying convergence orders for different values of α and β with N = 100 for both L1 and $L2 - 1_{\sigma}$ schemes are listed. It is shown that $2 - \beta$ temporal accuracy has been reached for the L^2 -errors in case of L1 scheme (see section 1.5, chapter 1), while a high order of second temporal accuracy has been reached for the L^2 -errors in case $L2 - 1_{\sigma}$ scheme which accords with the temporal order of convergence provided by Theorem 4.2. Orders of spatial convergence are shown for various values of α values at $\tau = 1/500$ in figure 4.1. In addition, when the L^2 -errors diminish exponentially, spatial spectral accuracy increases for a smooth solution. The convergence findings coincide completely with the theoretical ones. At each level of convergence, we see full concordance between theoretical and experimental results.



Figure 4.1 – Rate of convergence in space direction for different values of α and β at $\tau = 1/500$.

Chapter 5 Software packages for the solutions of models described by fractional partial differential equations with delay

This chapter is devoted to describing the software package used in this dissertation for numerical methods of some models with fractional order and time delay effect. More precisely, we present here the main characteristics of the developed software complexes that allow modeling the impact of time and space fractional orders on the behavior of the dynamics for the solutions of nonlinear delay fractional models. In addition, the tools used in the complex, their main functions and components are described, and examples of the operation of the software package are considered. The theoretical basis of the complexes are numerical methods and algorithms developed to solve fractional models with delay. The computational experiments in chapters 1-4, were carried out using the software program described in this chapter. Four software packages have been developed corresponding to the described algorithm under study.

The software packages were written in the Wolfram Mathematica programming language (version: 12.1), which is quite intended for specialists in the field of mathematical modeling and numerical methods. The software program has passed the procedure of state registration of the computer program, the corresponding certificate has been obtained, see figure 5.8.

5.1 Main functions of the software packages

The software packages designed in Wolfram Mathematica have a modular structure and are designed to programmatically solve models described by fractional partial differential equations. More specifically, the developed software package includes four independent modules for modeling the impact of time and space fractional orders on the behavior of the dynamics for the solutions models which correspond to the following numerical schemes:

1. An explicit numerical scheme for the nonlinear time-space fractional order reaction-diffusion equations with delay.

- 2. An explicit numerical scheme for the generalized nonlinear multi-term time-space order fractional reaction-diffusion equation with delay.
- 3. An explicit numerical scheme for a generalized form of fractional-order Schnakenberg reaction-diffusion model with gene expression time delay.
- 4. High-order numerical scheme for the nonlinear time-space fractional order reaction-diffusion equations with delay.

5.2 Structure of the software packages

It is recommended that the system meet the following requirements for the purpose of software package implementation:

- Operating system: Microsoft Windows 10/Windows 7 Platform Update/Server 2016/Server 2019;
- Disk Space: Minimum 20 GB;
- Processor: x86-64 compatible CPU;
- System Memory (RAM): 4 GB and above;
- Graphics card: dual-precision graphics card that supports OpenCL or CUDA, such as many cards from NVIDIA, AMD, and others;
- Internet access: required in order to use online data sources from the Wolfram Knowledge base.

Since we construct an explicit method, so every later time step of a system depends on the state of the system at the current step time. Steps can be generally described as follows:

Step 1. A set of parameters must be identified in the code beginning, such as the temporal fractional order parameter β , the spatial fractional order parameter α , the spatial polynomial of degree N, the right and left boundaries of the domain of definition of the boundary value problem, given in time T and space Ω , the time step τ , the delay term s, the temporal mesh M, the Gamma function Γ and the exact solution or initial boundary conditions which already given.

Step 2. Define the space fractional derivative on the space interval, then determine the right-hand side function.

Step 3. Evaluation Legendre polynomials and their k - th derivatives up to degree n and determine the Gauss-Lobatto points and weights.

Step 4. Calculating the Mass M and the stiffness S matrices. which represents a system of linear equations that need to be solved to get the solutions. Step 5. Making the main loop and output.

As a result of the program, the user will receive a list of the errors and corresponding convergence orders. Additionally, graphs can be output which describe the impact of time and space fractional orders on the behavior of the dynamics for the approximate solutions. Based on the tasks imposed on the software package, its structure can be represented in the form of a modular architecture shown in figure 5.1.



Figure 5.1 - General scheme of the structure of the software package.

5.3 Examples of the software packages

Two examples here are presented to further show how the dynamics of the solution to delayed models described by fractional partial differential equations are affected by fractional orders in the temporal and spatial directions.

Example 5.1. We consider the following fractional problem, where the dynamics of the solution are very interesting and the exact solution is unknown [131]

$$\frac{\partial^{\beta}\Phi}{\partial t^{\beta}}(x,t) = \frac{\partial^{\alpha}\Phi}{\partial |x|^{\alpha}}(x,t) + \epsilon \Phi(x,t)(1 - \Phi(x,t))(1 + \Phi(x,t-1.5)), \qquad (5.1)$$

with the initial value $\Phi(x,0) = e^{-2x^2}$ and $x \in (a,b), t \in (0,3]$.

To solve this problem, we use the fully discrete L1-Galerkin spectral scheme (1.10) introduced in chapter 1, which copes with nonlinear time-space fractional order problems with delay.

We set the following parameters as:

- the temporal fractional order parameter $\beta = 0.8; 0.5; 0.2;$
- the spatial fractional order parameter $\alpha = 1.8; 1.5; 1.2;$
- the delay parameter s = 1.5;
- the space polynomial N = 100;
- the time step $\tau = 1.5/20;$
- $-M = \left\lceil \frac{3}{\tau} \right\rceil;$
- $-\epsilon = 0.1; 1$

Following that, applying the steps 2-5 until we reach to the main loop. In this step, the program will solve the linear system resulted from full discretization. We determine the out put data as graphs in order to describe the impact of time and space fractional orders on the behavior of the dynamics for the approximate solutions.

Figures 5.2-5.5 show the profiles of the numerical solution when the fractional order parameters α , β with $\epsilon = 0.1$ and 1. We can observe from these figures that the evolution of the solution is pretty sharp on the first time steps depending on β . We also find that the fractional-order parameter α affects the shape of the solutions. We can say that the fractional-order parameters can be used in physics to modify

α=1.8, *β*=0.8 *α*=1.5, *β*=0.8 *α*=1.2, *β*=0.8 u(x,t) 0.5} u(x,t) 0.5 u(x,t α=1.5, β=0.5 α=1.2, β=0.5 α=1.8, β=0.5 u(x,t) u(x,t) u(x,t) α=1.8, β=0.2 α=1.5, β=0.2 α=1.2, β=0.2 u(x,t) 0.5 u(x,t) u(x,t) 0.5 20

the shape of waves without changing the non-linearity and dispersion effects of the fractional nonlinear problems.

Figure 5.2 — Evaluations of Φ for different fractional order parameters α and ϵ with $\epsilon = 0.1$.



Figure 5.3 — Comparison of profiles of the approximate solutions for Example 5.1 at $\epsilon = 0.1$ and t = 3.

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Figure 5.4 — Evaluations of Φ for different fractional order parameters α and ϵ with $\epsilon = 1$.



Figure 5.5 — Comparison of profiles of the approximate solutions for Example 5.1 at $\epsilon = 1$ and t = 3.

Example 5.2. We consider the following fractional problem, where the dynamics of the solution are very interesting and the exact solution is unknown

$$\sum_{r=1}^{8} \frac{\partial^{\beta_r} \Phi}{\partial t^{\beta_r}}(x,t) = \frac{\partial^{\alpha} \Phi}{\partial |x|^{\alpha}}(x,t) + \Phi(x,t) \left(1 - \Phi(x,t)\right) \left(1 + \Phi(x,t-1.5)\right), \quad (5.2)$$

for each $x \in (a,b)$ and $t \in (0,3]$, with the initial value $\Phi(x,0) = e^{-2x^2}$ and $\beta_r = \frac{r}{10}$.

To solve this problem, we use the fully discrete L1-Galerkin spectral scheme (2.10) introduced in chapter 2, which copes with the generalized nonlinear multi--term time-space fractional reaction-diffusion equations with delay.

We set the following parameters as:

- the temporal fractional order parameter $\beta = 0.8; 0.5; 0.2;$
- the spatial fractional order parameter $\alpha = 1.8; 1.5; 1.2;$
- the delay parameter s = 1.5;
- $-\beta_r = r/10, r = 1, \dots, 8$
- the space polynomial N = 100;
- the time step $\tau = 1.5/500;$
- $-M = \left\lceil \frac{3}{\tau} \right\rceil;$

Following that, apply steps 2-5, until we reach the main loop. The program will solve the linear system resulting from full discretization in this step. We determine the output data as graphs to describe the impact of time and space fractional orders on the behavior of the dynamics for the approximate solutions.

Figures 5.6 and 5.7 show the profiles of the numerical solution with the fractional order parameters $\alpha = 1.2, 1.5, 1.8$ with N = 100 and $\tau = 1.5/500$. We can observe that the fractional order parameter α affects the shape of the solutions. we can say that the fractional order parameters can be used in physics to modify the shape of waves without changing the non-linearity and dispersion effects of the fractional nonlinear problems.


Figure 5.6 — Evaluations of Φ for different fractional-order parameters α .



Figure 5.7 – Evaluations of Φ at x = 0 and t = T for different fractional order parameters α .

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Figure 5.8 - Certificate of registration of the computer program

Conclusion

This dissertation is devoted to developing and investigating numerical techniques for solving fractional differential equations with nonlinear delay effects. These kinds of effects might frequently occur in realistic world, for instance, when modeling automatic control systems with feedback, population dynamics and modelling complex biological processes. The main results obtained in this dissertation can be outlined as follows:

- (i) Chapter one is devoted to investigating numerically how the nonlinear delay approximation impacts the convergence and stability of the numerical solution for time and space fractional subdiffusion equations involving a delay parameter. In clear sense, for the nonlinear time-space fractional reaction-diffusion equations with time delay, the construction of an explicit numerical method based on the uniform L1 scheme for temporal fractional operators and the Galerkin–Legendre spectral approximation for the spatial fractional operator is presented. The stability and convergence of semi and fully discrete schemes are investigated using the fractional Halanay and fractional Grönwall inequalities, respectively. It has been proved that the scheme is unconditionally stable and convergent with a $2 - \beta$ order for time if the solution is smooth enough and deteriorates to β order in case of a non-smooth solution. The exponential order of convergence is achieved for space due to the use of the Galerkin Legendre spectral scheme. The graded L1 scheme can be handled to keep $2 - \beta$ order in case of a non-smooth solution in time. This will be our future consideration. The prepared numerical experiments show satisfactory results in comparison to the theoretical findings.
- (ii) In Chapter two, we have constructed and analyzed a novel explicit finite difference/Galerkin-Legendre spectral scheme for generalized nonlinear multi-term Riesz-space and Caputo-time fractional reaction-diffusion equation with delay. Other words, an efficient hybrid numerical scheme based on the L1 difference formula for the temporal direction, and the Galerkin-Legendre spectral method for the spatial direction is developed. Using an appropriate form of discrete fractional Grönwall inequality, the stability and the convergence of the fully discrete scheme were investigated. We have proved that

the proposed method is stable and has a convergent order $2 - \beta_m$, in time, and an exponential rate of convergence in space. Moreover, high-order difference schemes can be handled to raise the temporal convergence order. This can be done by using the Alikhanov scheme [77]. Two numerical examples are given to show that the numerical results are consistent with theoretical ones in the case of the smoothness of the solution with respect to time and space.

- (iii) In Chapter three, a novel numerical algorithm for the generalized fractional Schnakenberg diffusion model with time delay parameter was developed and analyzed. The Schnakenberg model is well-known as an influential model that is used in a variety of biological processes. We have investigated the impact of the nonlinear delay approximation on the convergence and stability of the suggested numerical solution for the model under consideration. The numerical solutions for this model are obtained by constructing an efficient numerical algorithm mixes the L1 approximation side by side with the Legendre-Galerkin spectral method. Investigating the stability and convergence of the numerical scheme included using an appropriate type of discrete fractional Grönwall inequality. It is shown that the proposed method is unconditionally stable, converges exponentially fast in space, and converges in time with an order of $2 - \beta$. Utilizing the Galerkin–Legendre spectral technique results in the exponential order of convergence for the space direction. In the case of solution smoothness with respect to time and space, numerical examples are offered to show that they are consistent with theoretical ones. A challenge which will be a part of future work. This challenge is related to the time derivative discontinuities behaviour of the solutions of the equations at multiple points generated by time delay and the Caputo fractional derivative. The nonuniform mesh schemes can cope better in that case [188].
- (iv) In Chapter four, we developed high-order spectral Galerkin approach to handle the nonlinear fractional order reaction-diffusion equations with fixed delay. This approach accomplished by constructing an effective numerical algorithm that integrates the efficacy of $L2 - 1_{\sigma}$ type approximation side by side to the effectiveness of the Galerkin spectral Legendre technique. Other words, on a uniform mesh we used the $L2 - 1_{\sigma}$ difference formula and

the Legendre-Galerkin spectral technique for time and space discretizations, respectively. According to the literature overview, the majority of earlier research provided error estimates only in a limited (local) time period or when the numerical solution declines in time. However, we presented a theoretical analysis to obtain the optimal error estimates for the suggested scheme with no constraints compared to earlier studies, using the developed $L2 - 1_{\sigma}$ fractional Grönwall type inequality in discrete version. In the case of smooth solutions, the suggested scheme's convergence analysis was established, and it was demonstrated that the scheme under consideration is effective with second order precision in time and spectral accuracy in space. In the situation of a non-smooth solution in time, a high-order graded L2- 1_{σ} scheme can be dealt with using a non-uniform Alikhanov[83; 189] scheme to preserve the second order. Additionally, a more generic investigation for problem (4.1) is possible by replacing the fixed delay with a distributed one [190]. These preparations are meant to serve as a road map for future study. Finally, a numerical test is offered to demonstrate the effectiveness of the proposed scheme and show that is consistent with theoretical results.

Recommendations and future works

Possible applications of these findings include the development of software gatherings for the numerical modeling of various problems characterized by equations with fractional derivatives and the influence of delay in time. In light of this, investigation of multi-term time fractional order problems with multi-delay effects may be a promising area for future algorithm development research. These type of equations has the ability to represent many complicated multi-rate physical and biological processes in accurate sense. This kind of problems can be expressed as in the following form

$$\sum_{r=0}^{m} q_r \frac{\partial^{\beta} \Phi}{\partial t^{\beta}} = \kappa \frac{\partial^{\alpha} \Phi}{\partial |x|^{\alpha}} + f\left(\Phi(x,t), \Phi(x,t-s_1), \Phi(x,t-s_2), \cdots, \Phi(x,t-s_r)\right) + g(x,t), \quad x \in \Omega, \quad t \in I,$$

endowed with initial-boundary conditions of the form

$$\begin{cases} \Phi(x,t) = \psi(x,t), & x \in \Omega, \quad t \in [-s,0], \\ \Phi(a,t) = \Phi(b,t) = 0, \quad t \in I, \end{cases}$$

where $s = \max\{s_1, s_2, \dots, s_r\} > 0$. Another possible investigation of further research on the topic of the dissertation might focus on developing and studying numerical methods for solving fractional problems that exhibit a distributed delay effect in the following form

$$\frac{\partial^{\beta}\Phi}{\partial t^{\beta}} - \kappa \frac{\partial^{\alpha}\Phi}{\partial |x|^{\alpha}} = f\left(x, t, \Phi(x, t), \int_{t-s}^{t} g\left(s, t, \Phi(s, x)\right)\right), \quad x \in \Omega, \quad t \in I,$$

endowed with initial-boundary conditions of the form

$$\begin{cases} \Phi(x,t) = \psi(x,t), & x \in \Omega, \quad t \in [-s,0], \\ \Phi(a,t) = \Phi(b,t) = 0, \quad t \in I, \end{cases}$$

Biological and medical problems, as well as other real-world models, are common places to find this kind of research activity.

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