Novel analytical and numerical methods for solving fractional dynamical systems

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To my Mum and Dad
During the past three decades, the subject of fractional calculus (that is, calculus of integrals and derivatives of arbitrary order) has gained considerable popularity and importance, mainly due to its demonstrated applications in numerous diverse and widespread fields in science and engineering. For example, fractional calculus has been successfully applied to problems in system biology, physics, chemistry and biochemistry, hydrology, medicine, and finance. In many cases these new fractional-order models are more adequate than the previously used integer-order models, because fractional derivatives and integrals enable the description of the memory and hereditary properties inherent in various materials and processes that are governed by anomalous diffusion. Hence, there is a growing need to find the solution behaviour of these fractional differential equations. However, the analytic solutions of most fractional differential equations generally cannot be obtained. As a consequence, approximate and numerical techniques are playing an important role in identifying the solution behaviour of such fractional equations and exploring their applications.

The main objective of this thesis is to develop new effective numerical methods and supporting analysis, based on the finite difference and finite element methods, for solving time, space and time-space fractional dynamical systems involving fractional derivatives in one and two spatial dimensions. A series of five published papers and one manuscript in preparation will be
presented on the solution of the space fractional diffusion equation, space fractional advection-dispersion equation, time and space fractional diffusion equation, time and space fractional Fokker-Planck equation with a linear or non-linear source term, and fractional cable equation involving two time fractional derivatives, respectively.

One important contribution of this thesis is the demonstration of how to choose different approximation techniques for different fractional derivatives. Special attention has been paid to the Riesz space fractional derivative, due to its important application in the field of groundwater flow, system biology and finance. We present three numerical methods to approximate the Riesz space fractional derivative, namely the L1/ L2-approximation method, the standard/shifted Grünwald method, and the matrix transform method (MTM). The first two methods are based on the finite difference method, while the MTM allows discretisation in space using either the finite difference or finite element methods. Furthermore, we prove the equivalence of the Riesz fractional derivative and the fractional Laplacian operator under homogeneous Dirichlet boundary conditions – a result that had not previously been established. This result justifies the aforementioned use of the MTM to approximate the Riesz fractional derivative.

After spatial discretisation, the time-space fractional partial differential equation is transformed into a system of fractional-in-time differential equations. We then investigate numerical methods to handle time fractional derivatives, be they Caputo type or Riemann-Liouville type. This leads to new methods utilising either finite difference strategies or the Laplace transform method for advancing the solution in time.

The stability and convergence of our proposed numerical methods are also investigated. Numerical experiments are carried out in support of our theoretical analysis. We also emphasise that the numerical methods we develop are applicable for many other types of fractional partial differential equations.
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Statement of Original Authorship

The work contained in this thesis has not been previously submitted for a degree or diploma at any other higher education institution. To the best of my knowledge and belief, the thesis contains no material previously published or written by another person except where due reference is made.

Signature:  

Qianqian Yang

Date:  

xxv
CHAPTER 1

Introduction

1.1 Background

The concept of fractional calculus (that is, calculus of integrals and derivatives of arbitrary order) may be considered an old and yet novel topic. In fact, the concepts are almost as old as their more familiar integer-order counterparts. As early as 1695, when Leibniz and Newton had just been establishing standard calculus, Leibniz and L'Hôpital had correspondence where they discussed the meaning of the derivative of order one half. Since then, many famous mathematicians have worked on this and related questions, creating the field which is known today as fractional calculus. A list of mathematicians who have provided important contributions up to the middle of last century, includes Laplace, Fourier, Abel, Liouville, Riemann, Grünwald, Letnikov, Lévy, Marchaud, Erdélyi, and Riesz. However, for three centuries, the theory of fractional calculus was developed mainly as a purely theoretical field of mathematics.

The fractional calculus is also considered a novel topic, since it is only during the last three decades that it has been the subject of specialised conferences and treatises. This was stimulated by the fact that many important applications of fractional calculus have been found in
numerous diverse and widespread fields in science, engineering and finance. Many authors have pointed out that fractional derivatives and integrals are very suitable for modelling the memory and hereditary properties of various materials and processes that are governed by anomalous diffusion. This is the main advantage of fractional derivatives in comparison with classical integer-order models, in which such effects are neglected.

It was Ross who organised the first conference on fractional calculus and its applications at the University of New Haven in June 1974, and edited the proceedings [123]. For the first monograph on this subject, the merit is ascribed to Oldham and Spanier [114], who after a joint collaboration started in 1968, published a book devoted to fractional calculus in 1974. One of the most widely used works on the subject of fractional calculus is the book of Podlubny [116] published in 1999, which provides an overview of the basic theory of fractional differentiation, fractional-order differential equations, methods of their solution and applications. Some of the latest works especially on fractional models of anomalous kinetics of complex processes are the volumes edited by Carpinteri and Mainardi [19] in 1997 and by Hilfer [55] in 2000, the book by Zaslavsky [162] in 2005, the book by Kilbas, Srivastava and Trujillo [66] in 2006, and the book by Sabatier, Agrawal, Tenreiro Machado [127] in 2007. Indeed, in the mean time, numerous other works (books, edited volumes, and conference proceedings) have also appeared. These include (for example) the remarkably comprehensive encyclopaedic-type monograph by Samko, Kilbas and Marichev [129], which was published in Russian in 1987 and in English in 1993, and the book devoted substantially to fractional differential equations by Miller and Ross [111], which was published in 1993.

Transport phenomena in complex systems, such as random fractal structures, exhibit many anomalous features that are qualitatively different from the standard behaviour characteristics of regular systems [18], and hence the traditional partial differential equations may not be adequate for describing the underlying phenomena. Anomalous diffusion is a phenomenon strongly connected with the interactions within complex and non-homogeneous backgrounds. This phenomenon is observed in transport of fluid in porous media, in chaotic heat baths, amorphous semiconductors, particle dynamics inside polymer networks, two-dimensional rotating flows and also in econophysics [26]. In the case of fractals, such anomalies are due to the spatial complexity of the substrate, which imposes geometrical constraints on the transport process on all length scales. These constraints may be also seen as temporal correlations existing on
all time scales. Intensive analytical and numerical work has been performed in recent years to elucidate the unusual transport properties on fractal structures [44]. Much interest has been focused on understanding diffusion processes on such spatially correlated media. The non-homogeneities of the medium may alter the laws of Markov diffusion in a fundamental way. In particular, the corresponding probability density of the concentration field may have a heavier tail than the Gaussian density, and its correlation function may decay to zero at a much slower rate than the usual exponential rate of Markov diffusion, resulting in long-range dependence. This phenomenon is known as anomalous diffusion [110].

A major approach to anomalous diffusion is that of a continuous time random walk (CTRW), which has a long history of development. In the CTRW approach, the random motion is performed on a regular lattice, but the length of a jump and the waiting time between two successive jumps are assumed to be random and drawn from a probability density function. Different assumptions on this probability density function lead to a variety of fractional differential equations (FDE) such as the fractional heat equation [5], the fractional advection-dispersion equation [79], the fractional kinetic equation [160], the fractional Fokker-Planck equation (FFPE) [78], and the Riesz fractional kinetic equation [26].

In recent years, considerable interest in fractional differential equations has been stimulated by the applications that it finds in numerical analysis and in the different areas of physical and chemical processes and engineering, including fractal phenomena [110]. A physical-mathematical approach to anomalous diffusion [110] may be based on a generalised diffusion equation containing derivatives of fractional order in space, or time, or space-time. Such evolution equations imply for the flux a fractional Fick’s law that accounts for spatial and temporal non-locality. Fractional-order derivatives and integrals provide a powerful instrument for the description of memory and hereditary properties of different substances [116].

Fractional differential equations have been recently treated by a number of authors. The development and implementation of efficient and accurate numerical methods, and the rigorous theoretical analysis of fractional differential equations are both very difficult tasks, in particular for the cases of high dimensions, because the fractional differential equations involve a fractional-order derivative. Although some numerical methods for solving the space, or time, or time-space fractional partial differential equations have been proposed, many questions are
still open, especially for the cases of higher dimensions. A need therefore arises for developing new numerical methods and analysis techniques, in particular, for higher dimensional computational models.

1.2 Literature Review

In this section, the current state of knowledge in the application of fractional derivatives and the analytical and numerical approaches for solving fractional partial differential equations (FPDE) is explored.

1.2.1 Applications of fractional derivatives

The concept of fractional derivatives is by no means new. In fact, they are almost as old as their more familiar integer-order counterparts [111, 114, 116, 129]. Fractional derivatives have recently been successfully applied to problems in system biology [159], physics [11, 108, 110, 128, 160], chemistry and biochemistry [156], hydrology [13, 78, 79], medicine [69, 70, 130, 54, 99, 53], and finance [51, 120, 132, 148, 107].

In the area of physics, fractional kinetic equations of the diffusion, diffusion-advection, and Fokker-Planck type are presented as a useful approach for the description of transport dynamics in complex systems that are governed by anomalous diffusion and non-exponential relaxation patterns [110]. Metzler and Kalfet [110] derived these fractional equations asymptotically from basic random walk models, and from a generalised master equation. They presented an integral transformation between the Brownian solution and its fractional counterpart. Moreover, a phase space model was presented to explain the genesis of fractional dynamics in trapping systems. These issues make the fractional equation approach powerful. Their work demonstrates that fractional equations have come of age as a complementary tool in the description of anomalous transport processes.

Zaslavsky [160] reviewed a new concept of fractional kinetics for systems with Hamiltonian chaos. New characteristics of the kinetics are extended to fractional kinetics and the most important are anomalous transport, superdiffusion and weak mixing, amongst others. Different
important physical phenomena, including the cooling of particles and signals, particle and wave traps, and Maxwell’s Demon, for example, represent some domains where fractional kinetics prove to be valuable.

In the area of financial markets, fractional order models have been recently used to describe the probability distributions of log-prices in the long-time limit, which is useful to characterise the natural variability in prices in the long term. Meerschaert and Scalas [104] introduced a time-space fractional diffusion equation to model the CTRW scaling limit process densities when the waiting times and the log-returns are uncoupled (independent), and a coupled fractional diffusion equation if the waiting times and the log-returns are coupled (dependent).

In the area of medical imaging analysis, Hall and Barrick [53] recently pointed out that the model of restricted diffusion commonly employed in the analysis of diffusion MR data is not valid in complex environments, such as human brain tissue. They described an imaging method based on the theory of anomalous diffusion and showed that images based on environmental complexity may be constructed from diffusion-weighted MR images, where the anomalous exponent $\gamma < 1$ and fractal dimension $d_w$ are measured from diffusion-weighted MRI data.

In medicine, some authors have suggested that fractional models may be appropriate for modelling neuronal dynamics. If the ions are undergoing anomalous subdiffusion, it is suggested that comparison with models that assume standard or normal diffusion will likely lead to incorrect or misleading diffusion coefficient values [131]. A recent study on spiny Purkinje cell dendrites showed that spines trap and release diffusing molecules resulting in anomalously slow molecular diffusion along the dendrite [130]. Henry et al. [54] derived a fractional cable equation from the fractional Nernst-Planck equations to model anomalous electrodeffusion of ions in spiny dendrites. They subsequently found a fractional cable equation by treating the neuron and its membrane as two separate materials governed by separate fractional Nernst-Planck equations and employed a small ionic concentration gradient assumption [69, 70].

As far as the geometric and physical interpretations of fractional integration and differentiation are concerned, Podlubny [117] has devised a novel interpretation. In particular, he proposes a physical interpretation based on two kinds of time — cosmic time and individual time — and relates this interpretation to similar ideas used in the theory of relativity.
Fractional dynamical systems provide a powerful framework for the modelling of many dynamical processes. Therefore, it is important to identify their solution behaviours to enable their applications to be explored. In the next section, analytical solutions of FPDE are reviewed.

1.2.2 Existing analytical solution methods for FPDE

Fractional differential equations have been recently analysed by a number of authors, for example, Wyss [147] considered the time fractional diffusion equation and the solution is given in closed form in terms of Fox functions, and Schneider and Wyss [133] considered the time fractional diffusion and wave equations. The corresponding Green functions are obtained in closed form for arbitrary space dimensions in terms of Fox functions and their properties are exhibited.

Using the similarity method and the method of Laplace transform, Gorenflo et al. [47] proved that the scale-invariant solutions of the mixed problem of signaling type for the time-fractional diffusion-wave equation are given in terms of the Wright function in the case $0 < \alpha < 1$ and in terms of the generalised Wright function in the case $1 < \alpha < 2$. The reduced equation for the scale-invariant solutions is given in terms of the Caputo-type modification of the Erdelyi-Kober fractional differential operator.

Agrawal [1] considered a time fractional diffusion-wave equation in a bounded space domain. The fractional time derivative is described in the Caputo sense. Using the finite sine transform technique and the Laplace transform, the solution is expressed in terms of the Mittag-Leffler functions. Results showed that for fractional time derivatives of order $1/2$ and $3/2$, the system exhibits, respectively, slow diffusion and mixed diffusion-wave behaviours.

Liu et al. [79] considered the time-fractional advection-dispersion equation and derived the complete solution using variable transformation, Mellin and Laplace transforms, and properties of the H-function. Gorenflo et al. [50] derived the fundamental solution for the time fractional diffusion equation, and interpreted it as a probability density of a self-similar non-Markovian stochastic process related to the phenomenon of slow anomalous diffusion. Duan [33] derived the fundamental solution for time- and space-fractional partial differential equations in terms of Fox’s H-function.
Anh and Leonenko [6] considered scaling laws for fractional diffusion-wave equations with singular data. The Gaussian and non-Gaussian limiting distributions of the rescaled solutions of the fractional (in time) diffusion-wave equation for Gaussian and non-Gaussian initial data with long-range dependence are described in terms of multiple Wiener-Ito integrals. Anh and Leonenko [7] presented a spectral representation of the mean-square solution of the fractional diffusion equation with a random initial condition. Gaussian and non-Gaussian limiting distributions of the renormalised solution of the fractional-in-time and in-space kinetic equation are described in terms of multiple stochastic integral representations.

Orsingher and Beghin [12] considered and proved that the solutions to the Cauchy problem of the fractional telegraph equation can be expressed as the distribution of a suitable composition of different processes. Beghin and Orsingher [115] studied the fundamental solutions to time-fractional telegraph equations. They obtained the Fourier transform of the solutions for any $\alpha$ and gave a representation of their inverse, in terms of stable densities. For the special case $\alpha = 1/2$, they showed that the fundamental solution is the distribution of a telegraph process with Brownian time.

Huang and Liu [59] considered the time fractional diffusion equation with appropriate initial and boundary conditions in an $n$-dimensional whole-space and a half-space. Its solution has been obtained in terms of Green functions by Schneider and Wyss [133]. For the problem in whole-space, an explicit representation of the Green functions can also be obtained. However, an explicit representation of the Green functions for the problem in half-space is difficult to determine, except in the special cases $\alpha = 1$ with arbitrary $n$, or $n = 1$ with arbitrary $\alpha$. By investigating the explicit relationship between the Green functions of the problem with initial conditions in whole-space and that of the same problem with initial and boundary conditions in half-space, an explicit expression for the Green functions corresponding to the latter can be derived in terms of Fox functions. They also extended some results of Liu et al. [79] concerning the advection-dispersion equation and obtained its solution in a half-space and in a bounded space domain.

Huang and Liu [57] considered the space-time fractional advection-dispersion equation in which the first-order time derivative is replaced with a Caputo derivative of order $\alpha \in (0, 1]$, and the second-order space derivative is replaced with a Riesz-Feller derivative of order $\beta \in$
They derived the solution of its Cauchy problem in terms of the Green functions and the representations of the Green function by applying its Fourier-Laplace transforms. The Green function also can be interpreted as a spatial probability density function evolving in time. A similar approach was proposed for another kind of space-time fractional advection-dispersion equation whose space and time derivatives were both replaced with Caputo derivatives \([58]\).

Mainardi et al. \([101]\) considered the basic models for anomalous transport provided by the integral equation for a continuous time random walk (CTRW) and by the time fractional diffusion equation. They compared the corresponding fundamental solutions of these equations in order to investigate numerically the increasing quality of the approximation with advancing time.

Angulo et al. \([5]\) discussed fractional diffusion and fractional heat equations, where the diffusion operator is the composition of the Bessel and Riesz potentials. In the case of an unbounded spatial domain, a solution is formulated in terms of the Fourier transform of its spatially and temporally homogeneous Green function. The spectral density of the resulting solution is then obtained explicitly. The result implies that the solution of the fractional heat equation may possess spatial long-range dependence asymptotically. Mainardi et al. \([100]\) derived the fundamental solution of the space-time fractional diffusion equation. Metzler and Klafter \([110]\) studied the separation of variables for a fractional diffusion equation with a potential term, describing a generalisation of an escape problem through a fluctuating bottleneck. The results lead to a further understanding of the fractional framework in the description of complex systems that exhibit anomalous diffusion. Chen et al. \([23]\) derived the analytical solution for the time-fractional telegraph equation by the method of separation of variables. Luchko and Gorenflo \([97]\) developed an operational method for solving fractional differential equations with Caputo derivatives and the obtained solutions are expressed through Mittag-Leffler type functions.

However, the analytic solutions of most fractional differential equations are not usually expressed explicitly. As a consequence, many authors have discussed approximate solutions of the FPDE, which are reviewed in the next section.
1.2.3 Existing numerical methods for solving FPDE

To date most existing numerical solution techniques for equations involving fractional differential operators are based on random walk models [48, 49, 50, 52, 84, 91], the finite difference method [78, 106, 107, 135, 163, 142, 45, 164, 71, 157, 90, 26, 22, 76, 89, 165, 169, 136, 24, 149, 151, 150, 88], the finite element method [122, 41, 38, 39, 153], numerical quadrature [2, 67, 155], the method of Adomian decomposition [65, 112], Monte Carlo simulation [42, 102] or the newly proposed matrix transform method [60, 61, 62, 63, 152, 150, 149, 153]. Examples of random walk model methods include the work done by Gorenflo and Mainardi, who constructed random walk models for the space fractional diffusion processes [48] and the Lévy-Feller diffusion processes [49], based on the Grünwald-Letnikov discretisation of the fractional derivatives occurring in the spatial pseudo-differential operator. More recently, Gorenflo et al. [50, 52] considered the discrete random walk models for time, and time-space fractional diffusion equations.

Liu et al. [84] proposed an explicit finite-difference scheme for the time fractional diffusion equation (TFDE). They derived the scaling restriction of the stability and convergence of the discrete non-Markovian random walk approximation for TFDE in a bounded domain. Liu et al. [91] presented a random walk model for approximating a Lévy-Feller advection-dispersion process, governed by the Lévy-Feller advection-dispersion differential equation (LFADE). They showed that the random walk model converges to LFADE by use of a properly scaled transition to vanishing space and time steps. They proposed an explicit finite difference approximation (EFDA) for LFADE, resulting from the Grünwald-Letnikov discretisation of fractional derivatives. As a result of the interpretation of the random walk model, the stability and convergence of EFDA for LFADE in a bounded domain were discussed.

Finite difference schemes have tended to dominate the literature with regards to numerical methods. For space FPDEs, the use of finite different methods to discretise in space leads naturally to a method of lines approach for advancing the solution in time. Liu, Anh and Turner [78] proposed a computationally effective method of lines technique for solving space fractional partial differential equations. They transformed the space FPDE into a system of ordinary differential equations that was then solved using backward differentiation formulas.
Meerschaert and Tadjeran [106] developed practical numerical methods for solving the one-dimensional space fractional advection-dispersion equation with variable coefficients on a finite domain. The application of their results was illustrated by modelling a radial flow problem. The use of the fractional derivative allowed the model equations to capture the early arrival of a tracer observed at a field site. Zhang et al. [163] investigated a numerical approximation of the Lévy-Feller diffusion equation and gave its probabilistic interpretation. Ciesielski and Leszczynski [26] presented a numerical solution of the anomalous diffusion equation with the Riesz fractional derivative (ADE-RFD). Meerschaert and Tadjeran [107] examined some practical numerical methods to solve the case when a left-handed, or a right-handed fractional spatial derivative may be present in the partial differential equation and discussed the stability, consistency, and (therefore) convergence of the methods.

Other authors to have formally analysed the error properties of finite difference methods include Shen and Liu [135], who discussed an error analysis of an explicit finite difference approximation for the space fractional diffusion equation with insulated ends. Tadjeran et al. [142] examined a practical numerical method that is second-order accurate in time and in space to solve a class of initial-boundary value fractional diffusion equations with variable coefficients on a finite domain. An approach based on the classical Crank-Nicolson method combined with spatial extrapolation was used to obtain temporally and spatially second-order accurate numerical estimates. Stability, consistency, and (therefore) convergence of the method were also examined. Shen et al. [136] presented explicit and implicit difference approximations for the Riesz FADE with initial and boundary conditions on a finite domain, and derived the stability and convergence of their proposed numerical methods.

Finite difference methods are also applicable in the numerical solution of time FPDEs. Zhuang and Liu [164] analysed an implicit difference approximation for the time fractional diffusion equation, and discussed the stability and convergence of the method. Langlands and Henry [71] investigated the accuracy and stability of an implicit numerical scheme (L1 approximation) for solving the fractional sub-diffusion equation. However, the global accuracy of the implicit numerical scheme has not been derived and it seems that the unconditional stability for all $\gamma$ in the range $0 < \gamma \leq 1$ has not been established.
Yuste and Acedo [158] proposed an explicit finite difference method and a new von Neumann-type stability analysis for the fractional subdiffusion equation. However, they did not give the convergence analysis and pointed out that it is not such an easy task when implicit methods are considered. Yuste [157] proposed a weighted average finite difference method for fractional diffusion equations. Its stability is analysed by means of a recently proposed procedure akin to the standard von Neumann stability analysis.

Chen et al. [22] considered a fractional partial differential equation (FPDE) describing subdiffusion. An implicit difference approximation scheme (IDAS) for solving a FPDE was presented. They proposed a Fourier method for analysing the stability and convergence of the IDAS, derived the global accuracy of the IDAS, and discussed its solvability. Numerical examples were given to compare with the exact solution for the order of convergence, and to simulate the fractional dynamical systems. Chen et al. [24] also proposed three different implicit approximations for the time fractional Fokker-Planck equation and proved these approximations are unconditionally stable and convergent.

Diethelm, Ford and Freed [29] presented an Adams-type predictor-corrector method for the time FPDE. They also discussed several modifications of the basic algorithm designed to improve the performance of the method. In their later work [30], the authors presented a detailed error analysis, including error bounds under various assumptions on the equation.

Authors to have applied finite difference methods to solve time-space FPDEs include Liu et al. [89] who investigated a fractional order implicit finite difference approximation for the space-time fractional diffusion equation with initial and boundary values. Liu et al. [90] also investigated the stability and convergence of the difference methods for the space-time fractional advection-diffusion equation.

Gorenflo and Abdel-Rehim [45] discussed the convergence of the Grünwald-Letnikov scheme for a time-fractional diffusion equation in one spatial dimension. These difference schemes can also be interpreted as discrete random walks. Lin and Xu [76] constructed a stable and high order scheme to efficiently solve the time-fractional diffusion equation. The proposed method is based on a finite difference scheme in time and Legendre spectral methods in space. Stability and convergence of the method were rigorously established. Zhuang et al. [169] presented an implicit numerical method for the time-space fractional Fokker-Planck equation and discussed
its stability and convergence.

Podlubny et al. [118] presented a matrix approach for the solution of time- and space-fractional partial differential equations. The method is based on the idea of a net of discretisation nodes, where solutions at every desired point in time and space are found simultaneously by the solution of an appropriate linear system. The structure of the linear system, involving triangular strip matrices, is exploited in the numerical solution algorithm. Implementations in MATLAB are provided. ¹

Aside from discrete random walk approaches and the finite difference method, other numerical methods for solving the space or time, or space-time fractional partial differential equations have been proposed. Fix and Roop [41] proved existence and uniqueness of the least squares finite-element solution of a fractional order two-point boundary value problem. Optimal error estimates were proved for piecewise linear trial elements. Ervin and Roop [38] presented a theoretical framework for the Galerkin finite element approximation to the steady state fractional advection dispersion equation. Appropriate fractional derivative spaces were defined and shown to be equivalent to the usual fractional dimension Sobolev spaces $H^s$. Existence and uniqueness results were proven, and error estimates for the Galerkin approximation derived. More recently, Ervin and Roop [39] discussed the steady state fractional advection dispersion equation (FADE) on bounded domains in $\mathbb{R}^d$. Fractional differential and integral operators were defined and analysed. Appropriate fractional derivative spaces were defined and shown to be equivalent to the fractional dimensional Sobolev spaces. A theoretical framework for the variational solution of the steady state FADE was presented. Existence and uniqueness results were proven, and error estimates obtained for the finite element approximation.

Applications of fractional-order models to control theory were considered by Vinagre et al. in [146]. The authors presented both continuous and discrete integer-order approximations. In the continuous case, they utilised continued fraction expansions and interpolation techniques as well as curve-fitting techniques. In the discrete case, they utilised numerical integration combined with either power series expansion or continued fraction expansion.

Kumar and Agrawal [67] presented a numerical method for the solution of a class of FDEs for which there is a link between the FDE and a Volterra type integral equation. The FDEs are

¹The MATLAB code of this work can be found at http://www.mathworks.com/matlabcentral/fileexchange/authors/8245.
expressed as initial value problems involving the Caputo fractional derivative, and this allows the reduction to the Volterra type integral equation. The authors proposed using quadratic interpolation functions over three successive grid points, which allows the integrals to be computed, thereby yielding a system of algebraic equations to be solved. The scheme handles both linear and nonlinear problems.

Agrawal [2] revisited earlier work by Yuan and Agrawal [155] on a memory-free formulation (MFF) for the numerical solution of an FDE. The original MFF used Gauss-Laguerre quadrature to approximate the integral that appears in the definition of the Caputo fractional derivative. The new, modified MMF introduced a change of variable in the integration that overcome some of the limitations of the original formulation, by correctly computing initial compliance and more accurately simulating creep response over a much greater duration.

Jafari and Daftardar-Gejji [65] proposed an Adomian decomposition method for solving the linear/nonlinear fractional diffusion and wave equations. Momani and Odibat [112] developed two reliable algorithms, the Adomian decomposition method and variational iteration method, to construct numerical solutions of the space-time FADE in the form of a rapidly convergent series with easily computable components. However, they did not give its theoretical analysis.

Marseguerra and Zoia [102] and Fulger et al. [42] presented an alternative numerical solution strategy based on Monte Carlo simulations. In this method, they simulated the fractional kinetics equations via continuous-time random walks with different assumptions on the distributions of jumps in space and distributions of waiting times. However, one notes from Fulger et al. [42] that this strategy is rather computationally expensive.

Al-Khaled and Momani [3] gave an approximate solution for a fractional diffusion-wave equation using the decomposition method. Ilić et al. [60, 61] considered a fractional-in-space diffusion equation with homogeneous and nonhomogeneous boundary conditions in one dimension, respectively. They derived the analytic solutions by a spectral representation, and constructed numerical approximations by the matrix transform method (MTM), which is an exciting new method with great promise for higher dimensions.

Research on numerical methods for higher dimensional FPDEs has been limited to date. Roop [122] investigated the computational aspects of the Galerkin approximation using continuous piecewise polynomial basis functions on a regular triangulation of the bounded domain in $\mathbb{R}^2$. 

Meerschaert et al. [105] derived practical numerical methods to solve two-dimensional fractional dispersion equations with variable coefficients on a finite domain and obtained first order accuracy in space and time. Zhuang and Liu [165] proposed a finite difference approximation for the two-dimensional time fractional diffusion equation and discussed the convergence and stability of the numerical method. Tadjeran and Meerschaert [141] presented a second-order accurate numerical method for the two-dimensional fractional superdiffusive differential equation. This numerical method combined the alternating directions implicit (ADI) approach with a Crank-Nicolson discretisation and a Richardson extrapolation to obtain an unconditionally stable second-order accurate finite difference method. The stability and the consistency of the method were established. We are not aware of any other papers in the literature that investigate the numerical solution and associated error analysis for the FPDE in higher dimensions.

**Concluding Remarks:** This review of the applications of fractional derivatives and the solution techniques for FPDE is by no means comprehensive, but serves as a base to begin to identify the importance and challenges in constructing new numerical approximation schemes for solving FPDE. One notes from the above discussion that numerical methods for the fractional partial differential equation comprise a very new and fruitful research field. Although the majority of the previous research in this field has focused on one-dimensional problems, there are still many open questions. Furthermore, research on the numerical methods of the higher dimensional FPDE are limited to date. Therefore, this motivates us to consider effective numerical methods for the FPDE in both one and two dimensions.

### 1.3 Thesis Objectives

The primary objectives of this thesis are to

**Develop new efficient numerical methods based on finite difference and finite element discretisation techniques for solving the time, space and time-space fractional dynamical systems in one and two dimensions**

The numerical treatment of integral-order ordinary differential equations, using for example the Euler method, linear multi-step methods, or predictor-corrector methods, has had quite a well-developed theory. These methods have also been modified for solving fractional-order ordinary
differential equations via the fractional Euler method, fractional linear multi-step methods, and fractional predictor-corrector methods. The fractional method of lines for solving the space fractional diffusion equation was first proposed in [78]. In this method, one transforms the partial differential equation into a system of ordinary differential equations. Some efficient numerical methods for time or space, or space-time fractional differential equations have been proposed, utilising the finite difference method [78, 106, 107, 135, 163, 142, 45, 164, 71, 157, 90, 26, 22, 76, 89, 165, 169, 136, 24, 149, 151, 150, 88], the finite element method [122, 41, 38, 39, 153], numerical quadrature [2, 67, 155], the method of Adomian decomposition [65, 112] and the matrix transform method [60, 61, 62, 63, 152, 150, 149, 153]. In many applications, the fractional dynamical systems are complex, especially for high dimensional problems. These problems are still open, and it is therefore an important task for computational and applied mathematicians to develop novel and innovative numerical methods and analysis techniques to address the stability and convergence of these new numerical methods in one and higher dimensions. Each of these methods is adequately developed, well integrated and appropriate to the aims of this PhD project.

A recent investigation [150] has demonstrated the potential of the new matrix transform method for solving problems in higher dimensions. Therefore, it is proposed to investigate the suitability of this method for solving time-space fractional diffusion equations. Here, either the finite difference method (FDM) or the finite element method (FEM) can be used to generate a matrix representation $A$ of the Laplacian operator $-\Delta$, and then the matrix transform method can be used to approximate $(-\Delta)^{\gamma/2}$ by $A^{\gamma/2}$. This strategy produces a system of fractional-in-time differential equations. We then investigate numerical methods to handle time fractional derivatives, be they Caputo type or Riemann-Liouville type. This leads to new methods utilising either finite difference strategies or the Laplace transform method for advancing the solution in time.

**Derive analytical solutions for the fractional dynamical systems in one and two dimensions**

Another objective of this thesis is to derive the analytical solutions for some fractional dynamical systems in one and two dimensions. By doing so, we can ascertain the accuracy of our proposed numerical methods.
Analyse the accuracy, stability and convergence of these new numerical methods

Theoretical studies of the numerical methods and the error estimates of fractional-order partial differential equations are limited. Meerschaert and Tadjeran [106, 107] proposed finite difference approximations and some analysis techniques for the space fractional diffusion equation in one dimension. Liu et al. investigated the convergence and stability of the explicit and implicit difference approximations for the space fractional diffusion equation [135, 163], the time fractional diffusion equation [84, 165], and the space-time fractional diffusion equation in one dimension [89, 90], respectively. Langlands and Henry [71] proposed an explicit difference method and a new von Neumann-type stability analysis for fractional diffusion equations. However, they did not derive the global accuracy of the implicit numerical scheme and they have not been able to prove algebraically that their method is unconditionally stable for all fractional orders. In fact, based on the different fractional-order derivatives, it has been found that these existing numerical methods and the classical numerical analysis for integer-order differential equations are unsuitable for fractional-order differential equations. A need therefore arises for developing new analysis techniques for corresponding proposed numerical methods.

1.4 Thesis Outline

This thesis is presented by publications. Our original contribution to the literature is listed in five published papers and one manuscript in preparation. The outlines of these papers are given in the following subsections.

1.4.1 Chapter 2: Numerical methods for FPDE-RSFD

In this chapter, we present the work on the numerical methods for solving the fractional diffusion equation and the fractional advection-dispersion equation with Riesz space fractional derivatives. This work has been published in the following paper:

Statement of Joint Authorship

Qianqian Yang (Candidate) Proposed three new numerical schemes for solving the Riesz space fractional partial differential equations, proved the equivalence between the two fractional operators, developed the numerical codes in Fortran and MATLAB, interpreted the results, and wrote the manuscript.

Fawang Liu Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, proofread the manuscript and acted as the corresponding author.

Ian W. Turner Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

Paper Abstract

We consider the numerical solution of a fractional partial differential equation with Riesz space fractional derivatives (FPDE-RSFD) on a finite domain. Two types of FPDE-RSFD are considered: the Riesz fractional diffusion equation (RFDE) and the Riesz fractional advection-dispersion equation (RFADE). The RFDE is obtained from the standard diffusion equation by replacing the second-order space derivative with the Riesz fractional derivative of order \( \alpha \in (1, 2] \). The RFADE is obtained from the standard advection-dispersion equation by replacing the first-order and second-order space derivatives with the Riesz fractional derivatives of order \( \beta \in (0, 1) \) and of order \( \alpha \in (1, 2] \), respectively. Firstly, analytic solutions of both the RFDE and RFADE are derived. Secondly, three numerical methods are provided to deal with the Riesz space fractional derivatives, namely, the L1/L2-approximation method, the standard/shifted Grünwald method, and the matrix transform method (MTM). Thirdly, the RFDE and RFADE are transformed into a system of ordinary differential equations, which is then solved by the method of lines. Finally, numerical results are given, which demonstrate the effectiveness and convergence of the three numerical methods.

1.4.2 Chapter 3: Analytical and numerical solutions for TSS-FDE

In this chapter, we present the work on the analytical and numerical solutions for the time and space-symmetric fractional diffusion equation. This work has been published in the following paper:

Statement of Joint Authorship

Qianqian Yang (Candidate) Derived the analytical solution, proposed two new numerical schemes for solving the time and space-symmetric fractional diffusion equation, developed the numerical codes in Fortran and MATLAB, interpreted the results, wrote the manuscript, acted as the corresponding author, and presented the work at CTAC’08(Canberra).

Ian W. Turner Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

Fawang Liu Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

Paper Abstract

We consider a time and space-symmetric fractional diffusion equation (TSS-FDE) under homogeneous Dirichlet conditions and homogeneous Neumann conditions. The TSS-FDE is obtained from the standard diffusion equation by replacing the first-order time derivative by the Caputo fractional derivative of order $\alpha \in (0, 1)$, and the second order space derivative by the symmetric fractional derivative of order $\beta \in (1, 2]$. Firstly, a method of separating variables is used to express the analytical solution of the TSS-FDE in terms of the Mittag–Leffler function. Secondly, we propose two numerical methods to approximate the Caputo time fractional derivative, namely, the finite difference method and the Laplace transform method. The symmetric space fractional derivative is approximated using the matrix transform method. Finally, numerical results are presented to demonstrate the effectiveness of the numerical methods and to confirm the theoretical claims.

1.4.3 Chapter 4: Computationally efficient numerical methods for TSFFPE

In this chapter, we present the work on the numerical solutions for the time and space fractional Fokker-Planck equations. This work has been published in the following paper:

**Statement of Joint Authorship**

**Qianqian Yang** (Candidate) Proposed three new numerical schemes for solving the time and space fractional Fokker-Planck equations, developed the numerical codes in Fortran and MATLAB, interpreted the results, wrote the manuscript, acted as the corresponding author, and presented the work at FDA’08(Turkey).

**Fawang Liu** Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

**Ian W. Turner** Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

**Paper Abstract**

Fractional Fokker-Planck equations have been used to model several physical situations that present anomalous diffusion. In this paper, a class of time- and space-fractional Fokker-Planck equations (TSFFPE), which involve the Riemann-Liouville time fractional derivative of order $1 - \alpha$ ($\alpha \in (0, 1)$) and the Riesz space fractional derivative of order $\mu \in (1, 2)$, are considered. The solution of TSFFPE is important for describing the competition between subdiffusion and Lévy flights. However, effective numerical methods for solving TSFFPE are still in their infancy.

We present three computationally efficient numerical methods to deal with the Riesz space fractional derivative, and approximate the Riemann-Liouville time fractional derivative using the Grünwald method. The TSFFPE is then transformed into a system of ordinary differential equations (ODE), which is solved by the fractional implicit trapezoidal method (FITM). Finally, numerical results are given to demonstrate the effectiveness of these methods. These techniques can also be applied to solve other types of fractional partial differential equations.
1.4.4 Chapter 5: Stability and convergence of an ENM for TSFFPE-NST

In this chapter, we present the work on the stability and convergence analysis of a new numerical method for solving the time and space fractional Fokker-Planck equation with a nonlinear source term. This work has been published in the following paper:


Statement of Joint Authorship

Qianqian Yang (Candidate) Proposed a new numerical method for solving the time and space fractional Fokker-Planck equation with a nonlinear source term, conducted the stability and convergence analysis of the proposed method, developed the numerical codes in Fortran and MATLAB, interpreted the results, and wrote the manuscript.

Fawang Liu Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, proofread the manuscript, and acted as the corresponding author.

Ian W. Turner Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

Paper Abstract

Fractional Fokker-Planck equations (FFPE) have gained much interest recently for describing transport dynamics in complex systems that are governed by anomalous diffusion and non-exponential relaxation patterns. However, effective numerical methods and analytic techniques for the FFPE are still in their embryonic state. In this paper, we consider a class of time-space fractional Fokker-Planck equations with a nonlinear source term (TSFFPE-NST), which involve the Caputo time fractional derivative (CTFD) of order $\alpha \in (0, 1)$ and the symmetric Riesz space fractional derivative (RSFD) of order $\mu \in (1, 2]$. Approximating the CTFD and RSFD using the L1-algorithm and shifted Grünwald method, respectively, a computationally effective numerical method is presented to solve the TSFFPE-NST. The stability and convergence of the proposed numerical method are investigated. Finally, numerical experiments are carried out to support the theoretical claims.
1.4.5 Chapter 6: Two new implicit numerical methods for the fractional cable equation

In this chapter, we present the work on the stability and convergence analysis of two new implicit numerical methods for solving the fractional cable equation. This work has been published in the following paper:


Statement of Joint Authorship

**Fawang Liu** Proposed two new implicit numerical methods for the fractional cable equation, conducted the stability and convergence analysis of the proposed method, wrote the majority of the manuscript, proofread the manuscript, and acted as the corresponding author.

**Qianqian Yang** (Candidate) Developed the numerical codes in Fortran and MATLAB, interpreted the results, wrote the numerical results part of the manuscript, and proofread the manuscript.

**Ian W. Turner** Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

Paper Abstract

The cable equation is one of the most fundamental equations for modelling neuronal dynamics. Cable equations with fractional order temporal operators have been introduced to model electrotonic properties of spiny neuronal dendrites.

In this paper we consider the following fractional cable equation involving two fractional temporal derivatives:

\[
\frac{\partial u(x, t)}{\partial t} = D_t^{1-\gamma_1} \left( \kappa \frac{\partial^2 u(x, t)}{\partial x^2} \right) - \mu^2 D_t^{1-\gamma_2} u(x, t) + f(x, t),
\]
where \( 0 < \gamma_1, \gamma_2 < 1, \kappa > 0, \) and \( \mu \) are constants, and \( \_0D_t^{1-\gamma}u(x, t) \) is the Riemann-Liouville fractional partial derivative of order \( 1 - \gamma \). Two new implicit numerical methods with convergence order \( O(\tau + h^2) \) and \( O(\tau^2 + h^2) \) for the fractional cable equation are proposed respectively, where \( \tau \) and \( h \) are the time and space step sizes. The stability and convergence of these methods are investigated using the energy method. Finally, numerical results are given to demonstrate the effectiveness of both implicit numerical methods. These techniques can also be applied to solve other types of anomalous subdiffusion problems.

1.4.6 Chapter 7: Novel numerical methods for solving TSFDE-2D

In this chapter, we derived two novel numerical methods to solve the two-dimensional time-space fractional diffusion equation. This work is about to be submitted for review:


Statement of Joint Authorship

Qianqian Yang (Candidate) Proposed two novel numerical methods for solving the two-dimensional time-space fractional diffusion equation, developed the numerical codes in MATLAB, interpreted the results, and wrote the majority of manuscript.

Ian W. Turner Directed and guided the work, derived the error bounds for terminating subspace expansion, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

Fawang Liu Directed and guided the work, assisted with the interpretation of results and the preparation of the paper, and proofread the manuscript.

Milos Ilić Assisted with the derivation of the error bounds for terminating subspace expansion and the preparation of the paper, and proofread the manuscript.

Paper Abstract

In this paper, we consider a time-space fractional diffusion equation in two dimensions (TSFDE-2D) with homogeneous Dirichlet boundary conditions. The TSFDE-2D is obtained from the
standard diffusion equation by replacing the first-order time derivative with the Caputo fractional derivative $t_\gamma D^\gamma u$, $\gamma \in (0, 1)$, and the second order space derivatives with the fractional Laplacian $-(\Delta)^{\alpha/2}$, $\alpha \in (1, 2]$. Using the matrix transform method (MTM) proposed by Ilić, Liu, Turner, and Anh (2006, *Fractional Calculus and Applied Analysis*, 9, 333-349), we transform the TSFDE-2D into a time fractional differential system as

$$t_\gamma D^\gamma u = -K_\alpha A^{\alpha/2} u,$$

where $A$ is the approximate matrix representation of $(-\Delta)$. Traditional approximation of $A^{\alpha/2}$ requires diagonalisation of $A$, which is very time-consuming for large sparse matrices. The novelty of our proposed numerical schemes is that, using either the finite difference method or the Laplace transform method to approximate the Caputo time fractional derivative, the solution of the TSFDE-2D is written in terms of a matrix function vector product $f(A)b$ at each time step, where $b$ is a suitably defined vector. Depending on the method used to generate the matrix $A$, the product $f(A)b$ can be approximated using either the preconditioned Lanczos method or the M-Lanczos method, which are powerful techniques for solving large linear systems. Our numerical methods allow $A$ to be symmetric if generated from the finite difference method, or non-symmetric if generated from the finite element method. We give error bounds for the new methods and illustrate their roles in solving the TSFDE-2D. We also derive the analytical solution of the TSFDE-2D in terms of the Mittag–Leffler function. Finally, numerical results are presented to verify the proposed numerical solution strategies.

### 1.4.7 Chapter 8: Conclusions

In this chapter, the new contributions of the PhD work are outlined and the main conclusions drawn from the work are summarised. This chapter concludes with some recommendations for future research.
CHAPTER 2

Numerical methods for fractional partial differential equations with Riesz space fractional derivatives

2.1 Introduction

The concept of fractional derivatives is by no means new. In fact, they are almost as old as their more familiar integer-order counterparts [111, 114, 116, 129]. Recently, however, fractional derivatives have been successfully applied to problems in system biology [159], physics [11, 108, 110, 128, 160], chemistry and biochemistry [156], hydrology [13, 14, 78, 79], and finance [51, 120, 132, 148]. These new fractional-order models are more adequate than the previously used integer-order models, because fractional order derivatives and integrals enable the description of the memory and hereditary properties of different substances [116]. This is the most significant advantage of the fractional order models in comparison with integer order models, in which such effects are neglected. In the area of physics, fractional space derivatives are used to model anomalous diffusion or dispersion, where a particle spreads at a rate inconsistent with the classical Brownian motion model [110]. In particular, the Riesz fractional
derivative includes a left Riemann-Liouville derivative and a right Riemann-Liouville derivative that allow the modelling of flow regime impacts from either side of the domain [160]. The fractional advection-dispersion equation (FADE) is used in groundwater hydrology to model the transport of passive tracers carried by fluid flow in a porous medium [78, 112]. Benson et al. [13, 14] also studied the FADE for solute transport in a subsurface material. However, the analytical solutions of the fractional order partial differential equations are usually derived in terms of Green functions or Fox functions [55, 100], and hence are difficult to evaluate. Therefore, the numerical treatment and supporting analysis of fractional order differential equations has become a fruitful research topic that offers great potential.

A number of authors have discussed the numerical methods for solving the FADE with non-symmetric fractional derivatives. Liu et al. [79] considered the time FADE and the solution was obtained using a variable transformation, together with Mellin and Laplace transforms, and H-functions. Huang and Liu [57] also considered the space-time FADE and the solution was obtained in terms of Green functions and representations of the Green function by applying the Fourier-Laplace transforms. Meerschaert and Tadjeran [106] presented practical numerical methods to solve the one-dimensional space FADE with variable coefficients on a finite domain. Liu et al. [78] transformed the space fractional Fokker-Planck equation into a system of ordinary differential equations (method of lines), which was then solved using backward differentiation formulas. Momani and Odibat [112] developed two reliable algorithms, the Adomian decomposition method and variational iteration method, to construct numerical solutions of the space-time FADE in the form of a rapidly convergent series with easily computable components. However, they did not give its theoretical analysis. Liu et al. [91] proposed an approximation of the Lévy-Feller advection-dispersion process by employing random walk and finite difference methods.

The RFADE with a symmetric fractional derivative, namely the Riesz fractional derivative, was derived from the kinetics of chaotic dynamics by Saichev and Zaslavsky [128] and summarised by Zaslavsky [160]. Ciesielski and Leszczynski [26] presented a numerical solution for the RFADE (without the advection term) based on the finite difference method. Meerschaert and Tadjeran [107] proposed a shifted Grünwald estimate for the two-sided space fractional partial differential equation. Shen et al. [136] presented explicit and implicit difference approximations for the space RFADE with initial and boundary conditions on a finite domain, and derived
the stability and convergence of their proposed numerical methods. To the best knowledge of
the authors, there is no other research on the numerical treatment for the RFADE. This moti-
vates us to investigate computationally efficient numerical techniques for solving the RFADE.

In this paper, we consider the following fractional partial differential equation with the Riesz
space fractional derivatives (FPDE-RSFD):

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) + K_\beta \frac{\partial^\beta}{\partial |x|^\beta} u(x,t),$$

$$0 < t \leq T, \ 0 < x < L,$$  \hspace{1cm} (2.1)

subject to the boundary and initial conditions given by

$$u(0,t) = u(L,t) = 0,$$ \hspace{1cm} (2.2)

$$u(x,0) = g(x),$$ \hspace{1cm} (2.3)

where $u$ is, for example, a solute concentration; $K_\alpha$ and $K_\beta$ represent the dispersion coefficient
and the average fluid velocity. The Riesz space fractional derivatives of order $\alpha (1 < \alpha \leq 2)$
and $\beta (0 < \beta < 1)$ are defined respectively as

$$\frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) = -c_\alpha (0D_x^\alpha + x D_L^\alpha) u(x,t),$$ \hspace{1cm} (2.4)

$$\frac{\partial^\beta}{\partial |x|^\beta} u(x,t) = -c_\beta (0D_x^\beta + x D_L^\beta) u(x,t),$$ \hspace{1cm} (2.5)

where

$$c_\alpha = \frac{1}{2 \cos \left( \frac{\pi \alpha}{2} \right)}, \quad \alpha \neq 1, \quad c_\beta = \frac{1}{2 \cos \left( \frac{\pi \beta}{2} \right)}, \quad \beta \neq 1,$$

$$0D_x^\alpha u(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_0^x \frac{u(x,t) d\xi}{(x-\xi)^{\alpha-1}},$$

$$x D_L^\alpha u(x,t) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_0^L \frac{u(x,t) d\xi}{(\xi-x)^{\alpha-1}},$$

$$0D_x^\beta u(x,t) = \frac{1}{\Gamma(1-\beta)} \frac{\partial}{\partial x} \int_0^x \frac{u(x,t) d\xi}{(x-\xi)^{\beta}},$$

$$x D_L^\beta u(x,t) = -\frac{1}{\Gamma(1-\beta)} \frac{\partial}{\partial x} \int_x^L \frac{u(x,t) d\xi}{(\xi-x)^{\beta}}.$$
The fractional kinetic equation \((2.1)\) has a physical meaning (see \([128, 160]\) for further details). Physical considerations of a fractional advection-dispersion transport model restrict \(1 < \alpha \leq 2, 0 < \beta < 1\), and we assume \(K_\alpha > 0\) and \(K_\beta \geq 0\) so that the flow is from left to right. The physical meaning of using homogeneous Dirichlet boundary conditions is that the boundary is set far enough away from an evolving plume such that no significant concentrations reach that boundary \([105, 107]\). In the case of \(\alpha = 2\) and \(\beta = 1\), Eq. \((2.1)\) reduces to the classical advection-dispersion equation (ADE). In this paper, we only consider the fractional cases: when \(K_\beta = 0\), Eq. \((2.1)\) reduces to the Riesz fractional diffusion equation (RFDE) \([128]\); when \(K_\beta \neq 0\), the Riesz fractional advection-dispersion equation (RFADE) is obtained \([160]\).

There are different techniques for approximating different fractional derivatives \([114, 116, 129]\). To avoid confusion on this issue, we remark that it is essential to adopt the correct approximation for the corresponding definition of the fractional operator. One contribution of this paper is that we illustrate how to choose different techniques for different fractional derivatives. For simulation of the Riemann-Liouville fractional derivative, there exists a link between the Riemann-Liouville and Grünwald-Letnikov fractional derivatives. This allows the use of the Riemann-Liouville definition during problem formulation, and then the use of the Grünwald-Letnikov definition for obtaining the numerical solution \([116]\). When using the standard Grünwald approximation for the Riemann-Liouville fractional derivative, Meerschaert and Tadjeran \([106]\) found that the standard Grünwald approximation to discretise the fractional diffusion equation results in an unstable finite difference scheme regardless of whether the resulting finite difference method is an explicit or an implicit scheme. In order to show how to use the standard Grünwald approximation and shifted Grünwald approximation, we consider the RFADE \((2.1)\). We approximate the diffusion term by the shifted Grünwald method and approximate the advection term by the standard Grünwald method. In our opinion, this is a new and novel approach.

One will often see RFADE \((2.1)\) defined in terms of the fractional Laplacian operator as

\[
\frac{\partial u(x,t)}{\partial t} = -K_\alpha (\nabla^\alpha) u(x,t) - K_\beta (\nabla^\beta) u(x,t),
\]

(2.6)
and it is widely assumed that the Riesz fractional derivative \( \frac{\partial^{\alpha}}{\partial |x|^\alpha} \) and the fractional Laplacian operator \( (-\Delta)^{\alpha/2} \) are equivalent [48, 128, 160]. Another contribution of this paper is that we clarify the use of the two existing definitions of the fractional Laplacian operator in the literature. The first definition uses the Fourier transform on an infinite domain [129], with a natural extension to include finite domains when the function \( u(x,t) \) is subject to homogeneous Dirichlet boundary conditions. The second definition uses eigenfunction expansion on a finite domain [60]. We show that using the first definition, the operators \( \frac{\partial^{\alpha}}{\partial |x|^\alpha} \) and \( (-\Delta)^{\alpha/2} \) are indeed equivalent. We also show that while the second definition is not mathematically equivalent, it can nonetheless be used to derive useful numerical approximations.

We propose two numerical methods to approximate the Riesz fractional derivative \( \frac{\partial^{\alpha}}{\partial |x|^\alpha} \): the standard/shifted Grünwald method and the L1/L2 approximation. For the fractional Laplacian \( (-\Delta)^{\alpha/2} \) defined using eigenfunction expansion we derive the analytic solutions of the RFDE and RFADE using a spectral representation, and develop the matrix transform method (MTM) to solve the RFDE and RFADE. Again, we emphasise that although the definitions of these operators are not equivalent, the numerical results show that all three methods are still effective at approximating the Riesz fractional derivative.

After introducing the three numerical methods to approximate the Riesz fractional derivative, we use the fractional method of lines proposed by Liu et al. [78] to transform the RFDE and RFADE into a system of time ordinary differential equations (TODEs). Then, the TODE system is solved using a differential/algebraic system solver (DASSL) [17].

The rest of this paper is organised as follows. Section 2.2 presents some important definitions and lemmas used in this paper. Analytic and numerical solutions for the RFDE and RFADE are derived in Sections 2.3 and 2.4, respectively. Section 2.5 provides the numerical results for solving the RFDE and RFADE. Finally, the main results are summarised in Section 2.6.

### 2.2 Preliminary knowledge

In this section, we outline important definitions and a lemma used throughout the remaining sections of this paper.

**Definition 2.1.** [48, 129] The Riesz fractional operator for \( n - 1 < \alpha \leq n \) on a finite interval
0 \leq x \leq L is defined as
\[
\frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) = -c_\alpha (0D^\alpha_x + xD^\alpha_\infty) u(x,t)
\]

where
\[
c_\alpha = \frac{1}{2 \cos \left( \frac{\pi \alpha}{2} \right)}, \quad \alpha \neq 1,
\]
\[
0D^\alpha_x u(x,t) = \frac{1}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_0^x \frac{u(\xi,t) d\xi}{(x-\xi)^{n+1-\alpha}},
\]
\[
xD^\alpha_\infty u(x,t) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_x^\infty \frac{u(\xi,t) d\xi}{(\xi-x)^{n+1-\alpha}}.
\]

**Lemma 2.1.** For a function \(u(x)\) defined on the infinite domain \([-\infty < x < \infty]\), the following equality holds
\[
-(-\Delta)^{\frac{\alpha}{2}} u(x) = -\frac{1}{2 \cos \left( \frac{\pi \alpha}{2} \right)} \left[ 0D^\alpha_x u(x) + xD^\alpha_\infty u(x) \right] = \frac{\partial^\alpha}{\partial |x|^\alpha} u(x).
\]

**Proof.** According to Samko et al. [129], a fractional power of the Laplace operator is defined as follows:
\[
-(-\Delta)^{\frac{\alpha}{2}} u(x) = -\mathcal{F}^{-1} |x|^\alpha \mathcal{F} u(x).
\] (2.7)

where \(\mathcal{F}\) and \(\mathcal{F}^{-1}\) denote the Fourier transform and inverse Fourier transform of \(u(x)\), respectively. Hence, we have
\[
-(-\Delta)^{\frac{\alpha}{2}} u(x) = -\frac{1}{2 \pi} \int_{-\infty}^{\infty} e^{-i\xi \eta} |\xi|^\alpha \int_{-\infty}^{\infty} e^{i\xi \eta} u(\eta) d\eta d\xi.
\]

Supposing that \(u(x)\) vanishes at \(x = \pm \infty\), we perform integration by parts,
\[
\int_{-\infty}^{\infty} e^{i\xi \eta} u(\eta) d\eta = -\frac{1}{i \xi} \int_{-\infty}^{\infty} e^{i\xi \eta} u'(\eta) d\eta.
\]

Thus, we obtain
\[
-(-\Delta)^{\frac{\alpha}{2}} u(x) = -\frac{1}{2 \pi} \int_{-\infty}^{\infty} u'(\eta) \left[ i \int_{-\infty}^{\infty} e^{i\xi(\eta-x)} |\xi|^\alpha \frac{d\xi}{\xi} \right] d\eta.
\]
Let \( I = i \int_{-\infty}^{\infty} e^{i\xi(y-x)} \frac{\xi^\alpha}{\xi} d\xi \), then
\[
I = i \left[ -\int_0^\infty e^{i\xi(x-\eta)} \xi^{\alpha-1} d\xi + \int_0^\infty e^{i\xi(y-x)} \xi^{\alpha-1} d\xi \right].
\]

Noting that
\[
L(t^{v-1}) = \int_0^\infty e^{-st} t^{v-1} dt = \frac{\Gamma(v)}{s^v}, \quad Re(v) > 0,
\]
for \( 0 < \alpha < 1 \), we have
\[
I = i \left[ -\Gamma(\alpha) \frac{\Gamma(\alpha)}{i(x-\eta)^\alpha} + \frac{\Gamma(\alpha)}{i(\eta-x)^\alpha} \right] = \text{sign}(x-\eta) \Gamma(\alpha) \Gamma(1-\alpha) \left[ i^{\alpha-1} + (-i)^{\alpha-1} \right].
\]

Using \( \Gamma(\alpha) \Gamma(1-\alpha) = \frac{\pi}{\sin \pi\alpha} \) and \( i^{\alpha-1} + (-i)^{\alpha-1} = 2 \sin \frac{\pi \alpha}{2} \), we obtain
\[
I = \frac{\text{sign}(x-\eta) \pi}{\cos \frac{\pi \alpha}{2} |x-\eta|^\alpha \Gamma(1-\alpha)}.
\]

Hence, for \( 0 < \alpha < 1 \),
\[
(-\Delta)^2 u(x) = -\frac{1}{2\pi} \int_{-\infty}^\infty u'(\eta) \frac{\text{sign}(x-\eta) \pi}{\cos \frac{\pi \alpha}{2} |x-\eta|^\alpha \Gamma(1-\alpha)} d\eta
\]
\[
= -\frac{1}{2 \cos \frac{\pi \alpha}{2}} \left[ \frac{1}{\Gamma(1-\alpha)} \int_{-\infty}^x u'(\eta) \eta^\alpha d\eta - \frac{1}{\Gamma(1-\alpha)} \int_x^\infty u'(\eta) (\eta-x)^\alpha d\eta \right].
\]

Following [116], for \( 0 < \alpha < 1 \), the Grünwald-Letnikov fractional derivative in \([a, x]\) is given by
\[
aD^\alpha_x u(x) = \frac{u(a)(x-a)^{-\alpha}}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(1-\alpha)} \int_a^x \frac{u'(\eta)}{(x-\eta)^\alpha} d\eta.
\]

Therefore, if \( u(x) \) tends to zero for \( a \to -\infty \), then we have
\[
-aD^\alpha_x u(x) = \frac{1}{\Gamma(1-\alpha)} \int_{-\infty}^x \frac{u'(\eta)}{(x-\eta)^\alpha} d\eta.
\]

Similarly, if \( u(x) \) tends to zero for \( b \to \infty \), then we have
\[
bD^\alpha_x u(x) = \frac{-1}{\Gamma(1-\alpha)} \int_x^\infty \frac{u'(\eta)}{(\eta-x)^\alpha} d\eta.
\]

Hence, if \( u(x) \) is continuous and \( u'(x) \) is integrable for \( x \geq a \), then for every \( \alpha \) (\( 0 < \alpha < 1 \)),
the Riemann-Liouville derivative exists and coincides with the Grünwald-Letnikov derivative. Finally, for $0 < \alpha < 1$, we have

$$-(\Delta)_{\alpha}^{\frac{1}{2}} u(x) = -\frac{1}{2 \cos \frac{\pi \alpha}{2}} [-\infty D_{x}^{\alpha} u(x) + x D_{\infty}^{\alpha} u(x)] = \frac{\partial^{\alpha}}{\partial |x|^{\alpha}} u(x),$$

where

$$-\infty D_{x}^{\alpha} u(x) = \frac{1}{\Gamma(1 - \alpha)} \frac{\partial}{\partial x} \int_{-\infty}^{x} \frac{u(\eta) d\eta}{(x - \eta)^{\alpha}},$$

$$x D_{\infty}^{\alpha} u(x) = -\frac{1}{\Gamma(1 - \alpha)} \frac{\partial}{\partial x} \int_{x}^{\infty} \frac{u(\eta) d\eta}{(\eta - x)^{\alpha}}.$$

Next, we present a similar derivation for the case of $1 < \alpha < 2$. Supposing that $u(x)$ and $u'(x)$ vanish at $x = \pm \infty$, we perform integration by parts twice, to obtain

$$\int_{-\infty}^{\infty} e^{ix\xi} u(\eta) d\eta = -\xi^{-2} \int_{-\infty}^{\infty} e^{ix\xi} u''(\eta) d\eta.$$

Hence, we have

$$-(\Delta)_{\alpha}^{\frac{1}{2}} u(x) = \frac{1}{2 \pi} \int_{-\infty}^{\infty} e^{-i\xi(x-\eta)} [\xi^{\alpha} u''(\eta)] d\xi = \frac{1}{2 \pi} \int_{-\infty}^{\infty} u''(\eta) \left[ \int_{-\infty}^{\infty} e^{i\xi(x-\eta)} |\xi|^{\alpha-2} d\xi \right] d\eta.$$

Let $I = \int_{-\infty}^{\infty} e^{i\xi(x-\eta)} |\xi|^{\alpha-2} d\xi$, then

$$I = \int_{0}^{\infty} e^{i\xi(x-\eta)} \xi^{\alpha-2} d\xi + \int_{0}^{\infty} e^{i\xi(x-\eta)} \xi^{\alpha-2} d\xi.$$

Noting that

$$\mathcal{L}(t^{\alpha-2}) = \int_{0}^{\infty} e^{-st} t^{\alpha-2} dt = \frac{\Gamma(v-1)}{s^{\alpha-1}}, \quad Re(v) > 1,$$

we have

$$I = \frac{\Gamma(\alpha - 1)}{|i(\eta - x)|^{\alpha-1}} + \frac{\Gamma(\alpha - 1)}{|i(x - \eta)|^{\alpha-1}} = \frac{\Gamma(\alpha - 1)\Gamma(2 - \alpha)}{|x - \eta|^{\alpha-1}\Gamma(2 - \alpha)} [i^{\alpha-1} + (-i)^{\alpha-1}].$$

Using $\Gamma(\alpha - 1)\Gamma(2 - \alpha) = \frac{\pi}{\sin \pi(\alpha-1)} = \frac{-\pi}{\sin \pi(\alpha)}$ and $i^{\alpha-1} + (-i)^{\alpha-1} = 2 \sin \frac{\pi \alpha}{2}$, we have

$$I = \frac{-\pi}{\cos \frac{\pi \alpha}{2} |x - \eta|^{\alpha-1}\Gamma(2 - \alpha)}.$$
2.2 Preliminary knowledge

Hence, for $1 < \alpha < 2$,

$$-(-\Delta)^{\frac{\alpha}{2}} u(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} u''(\eta) \frac{e^{-\pi\eta}}{\cos \frac{\pi\alpha}{2} |x - \eta|^{\alpha-1}} \Gamma(2 - \alpha) d\eta$$

$$= -\frac{1}{2\cos \frac{\pi\alpha}{2}} \left[ \frac{1}{\Gamma(2 - \alpha)} \int_{-\infty}^{x} \frac{u''(\eta)}{(x - \eta)^{\alpha-1}} d\eta + \frac{1}{\Gamma(2 - \alpha)} \int_{x}^{\infty} \frac{u''(\eta)}{(\eta - x)^{\alpha-1}} d\eta \right].$$

Following [116], for $1 < \alpha < 2$, the Gr"unwald-Letnikov fractional derivative in $[a, x]$ is given by

$$a D^\alpha_x u(x) = \frac{u(a)(x - a)^{-\alpha}}{\Gamma(1 - \alpha)} + \frac{u'(a)(x - a)^{1-\alpha}}{\Gamma(2 - \alpha)} + \frac{1}{\Gamma(2 - \alpha)} \int_{a}^{x} \frac{u''(\eta)}{(x - \eta)^{\alpha-1}} d\eta.$$

Therefore, if $u(x)$ and $u'(x)$ tend to zero for $a \to -\infty$, then we have

$$-\infty D^\alpha_x u(x) = \frac{1}{\Gamma(2 - \alpha)} \int_{a}^{x} \frac{u''(\eta)}{(x - \eta)^{\alpha-1}} d\eta.$$

Similarly, if $u(x)$ and $u'(x)$ tend to zero for $b \to \infty$, then we have

$$x D^\alpha_\infty u(x) = \frac{1}{\Gamma(2 - \alpha)} \int_{x}^{\infty} \frac{u''(\eta)}{(\eta - x)^{\alpha-1}} d\eta.$$

Hence, if $u(x)$ and $u'(x)$ are continuous and $u''(x)$ is integrable for $x \geq a$, then for every $\alpha$ ($1 < \alpha < 2$), the Riemann-Liouville derivative exists and coincides with the Gr"unwald-Letnikov derivative. Finally, for $1 < \alpha < 2$, we have

$$-(-\Delta)^{\frac{\alpha}{2}} u(x) = -\frac{1}{2\cos \frac{\pi\alpha}{2}} [-\infty D^\alpha_x u(x) + x D^\alpha_\infty u(x)] = \frac{\partial^\alpha}{\partial |x|^\alpha} u(x),$$

where

$$-\infty D^\alpha_x u(x) = \frac{1}{\Gamma(2 - \alpha)} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{x} \frac{u(\eta)d\eta}{(x - \eta)^{\alpha-1}},$$

$$x D^\alpha_\infty u(x) = \frac{1}{\Gamma(2 - \alpha)} \frac{\partial^2}{\partial x^2} \int_{x}^{\infty} \frac{u(\eta)d\eta}{(\eta - x)^{\alpha-1}}.$$

Further, if $n - 1 < \alpha < n$, then

$$-(-\Delta)^{\frac{\alpha}{2}} u(x) = -\frac{1}{2\cos \frac{\pi\alpha}{2}} [-\infty D^\alpha_x u(x) + x D^\alpha_\infty u(x)] = \frac{\partial^\alpha}{\partial |x|^\alpha} u(x),$$
where
\[-\infty D_\alpha^x u(x) = \frac{1}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_{-\infty}^{x} \frac{u(\eta) d\eta}{(x-\eta)^{\alpha+1-n}},\]
\[x D_\alpha^\infty u(x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_{x}^{\infty} \frac{u(\eta) d\eta}{(\eta-x)^{\alpha+1-n}}.\]

**Remark 2.1.** For a function \(u(x)\) given in a finite interval \([0, L]\), the above equality also holds by setting
\[u^*(x) = \begin{cases} 
  u(x) & x \in (0, L), \\
  0 & x \notin (0, L),
\end{cases}\]
i.e., \(u^*(x) = 0\) on the boundary points and beyond the boundary points.

**Definition 2.2.** [61] Suppose the Laplacian \((-\Delta)\) has a complete set of orthonormal eigenfunctions \(\varphi_n\) corresponding to eigenvalues \(\lambda_n^2\) on a bounded region \(\mathcal{D}\), i.e., \((-\Delta)\varphi_n = \lambda_n^2 \varphi_n\) on a bounded region \(\mathcal{D}\); \(\mathcal{B}(\varphi) = 0\) on \(\partial \mathcal{D}\), where \(\mathcal{B}(\varphi)\) is one of the standard three homogeneous boundary conditions. Let
\[\mathcal{F}_\gamma = \{ f = \sum_{n=1}^{\infty} c_n \varphi_n, \ c_n = \langle f, \varphi_n \rangle, \ \sum_{n=1}^{\infty} |c_n|^2 |\lambda_n^\gamma| < \infty, \ \gamma = \max(\alpha, 0) \} ,\]
then for any \(f \in \mathcal{F}_\gamma\), \((-\Delta)_{\alpha/2}\) is defined by
\[(-\Delta)_{\alpha/2} f = \sum_{n=1}^{\infty} c_n (\lambda_n^2)^{\alpha/2} \varphi_n.\]

### 2.3 Analytic solution and numerical methods of the RFDE

In this section, we consider the following Riesz fractional diffusion equation (RFDE)
\[
\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t), \quad 0 < t \leq T, \quad 0 < x < L, \quad 1 < \alpha \leq 2 \tag{2.8}
\]
with the boundary and initial conditions given by
\[u(0,t) = u(L,t) = 0, \quad (2.9)\]
\[u(x,0) = g(x). \quad (2.10)\]
We assume that \( u(x, t) \) and \( g(x) \) are both real-valued and sufficiently well-behaved functions. Firstly, we derive the analytic solution of the RFDE (2.8) based on Definition 2.2 in Section 2.3.1, and then introduce three different numerical methods for solving the RFDE (2.8) in Sections 2.3.2-2.3.4.

### 2.3.1 Analytic solution for the RFDE

In this subsection, we present a spectral representation for the RFDE (2.8) based on Definition 2.2 on a finite domain \([0, L]\) with homogeneous Dirichlet boundary conditions.

The spectral representation of the Laplacian operator \((-\Delta)\) is obtained by solving the eigenvalue problem:

\[
-\Delta \varphi = \lambda \varphi, \\
\varphi(0) = \varphi(L) = 0.
\]

The eigenvalues are \( \lambda_n = \frac{n^2 \pi^2}{L^2} \) for \( n = 1, 2, \ldots \), and the corresponding eigenfunctions are nonzero constant multiples of \( \varphi_n(x) = \sin\left(\frac{n \pi x}{L}\right) \). Next, the solution is given by

\[
u(x, t) = \sum_{n=1}^{\infty} c_n(t) \sin\left(\frac{n \pi x}{L}\right),
\]

which automatically satisfies the boundary conditions (2.9). Using Definition 2.2 and substituting \( u(x, t) \) into Eq. (2.8), we obtain

\[
\sum_{n=1}^{\infty} \left\{ \frac{dc_n(t)}{dt} + K_\alpha(\lambda_n)^{\frac{\alpha}{2}} c_n(t) \right\} \sin\left(\frac{n \pi x}{L}\right) = 0.
\]

The problem for \( c_n(t) \) becomes a system of ordinary differential equations

\[
\frac{dc_n(t)}{dt} + K_\alpha(\lambda_n)^{\frac{\alpha}{2}} c_n(t) = 0,
\]

which has the general solution

\[
c_n(t) = c_n(0) \exp(-K_\alpha(\lambda_n)^{\frac{\alpha}{2}} t).
\]
To obtain \( c_n(0) \) we use the initial condition (2.10)

\[
 u(x, 0) = \sum_{n=1}^{\infty} c_n(0) \sin \left( \frac{n\pi x}{L} \right) = g(x),
\]

from which we deduce that

\[
 c_n(0) = \frac{2}{L} \int_0^L g(\xi) \sin \left( \frac{n\pi \xi}{L} \right) d\xi = b_n.
\]

With this choice of the coefficients we have the analytic solution of the RFDE (2.8) based on Definition 2.2:

\[
 u(x, t) = \sum_{n=1}^{\infty} b_n \sin \left( \frac{n\pi x}{L} \right) \exp \left( -K_\alpha \left( \frac{n^2\pi^2}{L^2} \right)^\alpha t \right). \tag{2.11}
\]

### 2.3.2 L2-approximation method for the RFDE

In this section, we provide a numerical solution of the RFDE (2.8) based on Definition 2.1 and Lemma 2.1 by the L2-approximation method. In Section 2.2, the Riesz fractional derivative of order \( 1 < \alpha \leq 2 \) on a finite interval \([0, L]\) was defined in the sense of the Riemann-Liouville definition. There is another very important definition for the fractional derivative, namely, the Grünwald-Letnikov definition. For \( 1 < \alpha \leq 2 \), the left- and right-handed Grünwald-Letnikov fractional derivatives on \([0, L]\) are, respectively, given by

\[
 0D_x^\alpha u(x) = \frac{u(0)x^{-\alpha}}{\Gamma(1-\alpha)} + \frac{u'(0)x^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{1}{\Gamma(2-\alpha)} \int_0^x \frac{u^{(2)}(\xi)d\xi}{(x-\xi)^\alpha}, \tag{2.12}
\]

\[
x D_x^\alpha u(x) = \frac{u(L)(L-x)^{-\alpha}}{\Gamma(1-\alpha)} + \frac{u'(L)(L-x)^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{1}{\Gamma(2-\alpha)} \int_x^L \frac{u^{(2)}(\xi)d\xi}{(\xi-x)^\alpha}. \tag{2.13}
\]

Following [116], there exists a link between these two approaches to differentiation of arbitrary real order. Let us suppose that the function \( u(x) \) is \( n-1 \) times continuously differentiable in the interval \([0, L]\) and that \( u^{(n)}(x) \) is integrable in \([0, L]\). Then for every \( \alpha \) (\( 0 \leq n-1 < \alpha < n \)) the Riemann-Liouville derivative exists and coincides with the Grünwald-Letnikov derivative. This relationship between the Riemann-Liouville and Grünwald-Letnikov definitions allows the use of the Riemann-Liouville definition during the problem formulation, and then the Grünwald-Letnikov definition for obtaining the numerical solution [78]. Therefore, using the link between these two definitions and the L2-algorithm proposed by [78, 114], we can easily obtain the
following numerical discretisation scheme for the RFDE.

Assume that the spatial domain is \([0, L]\). The mesh is \(N\) equal intervals of \(h = L/N\) and \(x_l = lh\) for \(0 \leq l \leq N\).

The second term of the right-hand side of Eq. (2.12) can be approximated at \(x = x_l\) by

\[
\frac{u'(0)x_l^{1-\alpha}}{\Gamma(2 - \alpha)} \approx \frac{h^{-\alpha}}{\Gamma(2 - \alpha) l^{\alpha-1}}(u_1 - u_0).
\]

The third term of the right-hand side of Eq. (2.12) can be approximated at \(x = x_l\) by

\[
\frac{1}{\Gamma(2 - \alpha)} \int_0^{x_l} \frac{u^{(2)}(\xi)}{(x_l - \xi)^{\alpha-1}} d\xi = \frac{1}{\Gamma(2 - \alpha)} \sum_{j=0}^{l-1} \int_{jh}^{(j+1)h} \frac{u^{(2)}(x_l - \xi)}{\xi^{\alpha-1}} d\xi
\]

\[
\approx \frac{1}{\Gamma(2 - \alpha)} \sum_{j=0}^{l-1} \frac{u(x_l - (j-1)h) - 2u(x_l - jh) + u(x_l - (j+1)h)}{h^2} \int_{jh}^{(j+1)h} \frac{d\xi}{\xi^{\alpha-1}}
\]

\[
= \frac{h^{-\alpha}}{\Gamma(3 - \alpha)} \sum_{j=0}^{l-1} (u_{l-j+1} - 2u_{l-j} + u_{l-j-1})[(j + 1)^{2-\alpha} - j^{2-\alpha}],
\]

where \(u(x_l - jh) = u_{l-j}\).

Hence, we obtain an approximation of the left-handed fractional derivative (2.12) with \(1 < \alpha \leq 2\) as

\[
\alpha D_x^\alpha u(x_l) \approx \frac{h^{-\alpha}}{\Gamma(3 - \alpha)} \left\{ \frac{(1-\alpha)(2-\alpha)u_0}{l^\alpha} + \frac{(2-\alpha)(u_1 - u_0)}{l^{\alpha-1}} + \sum_{j=0}^{l-1} (u_{l-j+1} - 2u_{l-j} + u_{l-j-1})[(j + 1)^{2-\alpha} - j^{2-\alpha}] \right\}.
\]

Similarly, we can derive an approximation of the right-handed fractional derivative (2.13) with \(1 < \alpha \leq 2\) as

\[
x L \alpha D_x^\alpha u(x_l) \approx \frac{h^{-\alpha}}{\Gamma(3 - \alpha)} \left\{ \frac{(1-\alpha)(2-\alpha)u_N}{(N-l)^\alpha} + \frac{(2-\alpha)(u_N - u_{N-1})}{(N-l)^{\alpha-1}} + \sum_{j=0}^{N-l-1} (u_{l+j+1} - 2u_{l+j} + u_{l+j-1})[(j + 1)^{2-\alpha} - j^{2-\alpha}] \right\}.
\]

Therefore, using the fractional Grünwald-Letnikov definitions (2.12) and (2.13), together with
the numerical approximations (2.14) and (2.15), the RFDE (2.8) can be cast into the following system of time ordinary differential equations (TODEs):

\[
\frac{du_l}{dt} \approx - \frac{K_\alpha h^{-\alpha}}{2 \cos(\frac{\pi \alpha}{2}) \Gamma(3 - \alpha)} \left\{ \frac{(1 - \alpha)(2 - \alpha)u_0}{l^\alpha} + \frac{(2 - \alpha)}{l^{\alpha-1}} (u_1 - u_0) \right. \\
+ \sum_{j=0}^{l-1} (u_{l-j+1} - 2u_{l-j} + u_{l-j-1})[(j + 1)^{2-\alpha} - j^{2-\alpha}] \\
+ \frac{(1 - \alpha)(2 - \alpha)u_N}{(N - l)^\alpha} + \frac{(2 - \alpha)}{(N - l)^{\alpha-1}} (u_N - u_{N-1}) \\
+ \sum_{j=0}^{N-l-1} (u_{l+j-1} - 2u_{l+j} + u_{l+j+1})[(j + 1)^{2-\alpha} - j^{2-\alpha}] \left\}, \quad (2.16)
\]

where \( l = 1, \ldots, N - 1 \).

A number of efficient techniques for solving Eq.(2.16) have been previously proposed [17, 43, 77, 143]. Brenan et al. [17] developed the differential/algebraic system solver (DASSL), which is based on the backward differentiation formulas (BDF). DASSL approximates the derivatives using the \( k \)-th order BDF, where \( k \) ranges from one to five. At every step, it chooses the order \( k \) and step size based on the behaviour of the solution. In this work, we use DASSL as our TODE solver. This technique has been used by many researchers when solving adsorption problems involving step gradients in bidisperse solids [15, 80, 82], hyperbolic models of transport in bidisperse solids [83], transport problems involving steep concentration gradients [81], and modelling saltwater intrusion into coastal aquifers [85, 86].

### 2.3.3 Shifted Grünwald approximation method for the RFDE

The shifted Grünwald formula for discretising the two-sided fractional derivative is proposed by Meerschaert and Tadjeran [107], and it was shown that the standard (i.e., unshifted) Grünwald formula to discretise the fractional diffusion equation results in an unstable finite difference scheme regardless of whether the resulting finite difference method is an explicit or an implicit system. Hence, in this section, we discretise the Riesz fractional derivative \( \frac{\partial^\alpha}{\partial |x|^{\alpha}} u \) by the shifted Grünwald formulae [107]:

\[
0D^\alpha_x u(x_l) = \frac{1}{\pi^\alpha} \sum_{j=0}^{l+1} g_j u_{l-j+1} + O(h), \quad (2.17)
\]

\[
x D^\alpha_x u(x_l) = \frac{1}{\pi^\alpha} \sum_{j=0}^{N-l+1} g_j u_{l+j-1} + O(h), \quad (2.18)
\]
where the coefficients are defined by

\[ g_0 = 1, \quad g_j = (-1)^j \frac{(\alpha - 1) \ldots (\alpha - j + 1)}{j!} \]

for \( j = 1, 2, \ldots, N \). Then the RFDE (2.8) based on Definition 2.1 and Lemma 2.1 can be cast into the following system of time ordinary differential equations (TODEs):

\[
\frac{d u_l}{dt} \approx -\frac{K_\alpha}{2 \cos \left(\frac{\pi \alpha}{2}\right)} h^\alpha \left[ \sum_{j=0}^{l+1} g_j u_{l-j+1} + \sum_{j=0}^{N-l+1} g_j u_{l+j-1} \right], \quad (2.19)
\]

which can also be solved by DASSL.

### 2.3.4 Matrix transform method for the RFDE

Ilić et al. [60] proposed the matrix transform method (MTM) for a space fractional diffusion equation with homogeneous boundary conditions. They have shown that the MTM provides the best approximation to the analytic solution, because both the MTM and analytic solution are based on Definition 2.2. In this subsection, we apply this new technique to the RFDE (2.8) based on Definition 2.2. Following [60], we approximate the RFDE (2.8) by the matrix representation:

\[
\frac{dU}{dt} = -\eta A \hat{A} U, \quad (2.20)
\]

where \( \eta = \frac{K_\alpha}{h^{\alpha}} \), \( h \) is the discrete spatial step defined as \( h = \frac{L}{N} \), and \( U \in \mathbb{R}^{N-1}, A \in \mathbb{R}^{N-1 \times N-1} \) are given respectively by

\[
U = (u_1, \ldots, u_{N-1})^T, \quad (2.21)
\]

\[
A = \text{tridiag}(-1, 2, -1). \quad (2.22)
\]

The matrix \( A \) is symmetric positive definite (SPD), and therefore there exists a nonsingular matrix \( P \in \mathbb{R}^{N-1 \times N-1} \) such that

\[
A = P \Lambda P^T,
\]
where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{N-1})$, $\lambda_i (i = 1, 2, \ldots, N - 1)$ being the eigenvalues of $A$. Since the matrix $A$ is a symmetric tridiagonal matrix, eigenvalues $\lambda_i$ and eigenvector $P$ of $A$ could be easily obtained.

Hence, Eq. (2.20) becomes the following system of TODEs:

$$\frac{dU}{dt} = -\eta (P \Lambda^2 P^T) U,$$

and initially, we have

$$U(0) = [g(h), g(2h), \ldots, g((N - 1)h)]^T. \quad (2.24)$$

DASSL can again be used as the solver for this TODE system.

### 2.4 Analytic solution and numerical methods for the RFADE

In this section, we consider the following Riesz fractional advection-dispersion equation (RFADE):

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^{\alpha}}{\partial |x|^\alpha} u(x,t) + K_\beta \frac{\partial^{\beta}}{\partial |x|^\beta} u(x,t), \quad 0 < t \leq T, \quad 0 < x < L, \quad 1 < \alpha \leq 2, \quad 0 < \beta < 1, \quad (2.25)$$

with the boundary and initial conditions given by

$$u(0, t) = u(L, t) = 0, \quad (2.26)$$

$$u(x, 0) = g(x), \quad (2.27)$$

where $K_\alpha \neq 0, K_\beta \neq 0$. We assume that $u(x, t)$ and $g(x)$ are both real-valued and sufficiently well-behaved functions. Firstly, the analytic solution for the RFADE (2.25) based on Definition 2.2 is provided in Section 2.4.1, and then we introduce three different numerical methods for solving the RFADE (2.25) in Sections 2.4.2-2.4.4.
2.4 Analytic solution and numerical methods for the RFADE

2.4.1 Analytic solution for the RFADE

Using the Laplace and Fourier transforms, Shen et al. [136] derived the analytic solution for the RFADE (2.1) based on Definition 2.1 and Lemma 2.1 in terms of the Green function. In this subsection, we present a spectral representation for the RFADE (2.25) based on Definition 2.2 on a finite domain $[0, L]$ with homogeneous Dirichlet boundary conditions (2.26).

We set

$$u(x, t) = \sum_{n=1}^{\infty} c_n(t) \sin \left( \frac{n\pi x}{L} \right),$$

which automatically satisfies the boundary conditions (2.26). Using Definition 2.2 and substituting $u(x, t)$ into equation (2.25), we obtain

$$\sum_{n=1}^{\infty} \left\{ \frac{dc_n}{dt} + [K_\alpha (\lambda_n)^\alpha + K_\beta (\lambda_n)^\beta]c_n(t) \right\} \sin \left( \frac{n\pi x}{L} \right) = 0.$$

The problem for $c_n(t)$ becomes a system of ordinary differential equations

$$\frac{dc_n(t)}{dt} + [K_\alpha (\lambda_n)^\alpha + K_\beta (\lambda_n)^\beta]c_n(t) = 0,$$

which has the general solution

$$c_n(t) = c_n(0) \exp \left( - [K_\alpha (\lambda_n)^\alpha + K_\beta (\lambda_n)^\beta]t \right).$$

To obtain $c_n(0)$, we use the initial condition (2.27)

$$u(x, 0) = \sum_{n=1}^{\infty} c_n(0) \sin \left( \frac{n\pi x}{L} \right) = g(x),$$

which gives

$$c_n(0) = \frac{2}{L} \int_{0}^{L} g(\xi) \sin \left( \frac{n\pi \xi}{L} \right) d\xi = b_n.$$

Hence, the analytic solution of the RFADE (2.25) based on Definition 2.2 is given as:

$$u(x, t) = \sum_{n=1}^{\infty} b_n \sin \left( \frac{n\pi x}{L} \right) \exp \left( - [K_\alpha (\lambda_n)^\alpha + K_\beta (\lambda_n)^\beta]t \right),$$

where $\lambda_n = \frac{n^2 \pi^2}{L^2}$. 

$\Box$
2.4.2 L1- and L2-approximation method for the RFADE

In this subsection, we present a L1/L2 approximation method for the RFADE (2.25) based on Definition 2.1 and Lemma 2.1. We approximate the diffusion term by the L2-algorithm as presented in Section 2.3.2, and approximate the advection term by the L1-algorithm as follows.

For $0 < \beta < 1$, the left- and right-handed Grünwald-Letnikov fractional derivatives on $[0, L]$ are, respectively, given by

$$0D^\beta_x u(x) = \frac{u(0)x^{-\beta}}{\Gamma(1 - \beta)} + \frac{1}{\Gamma(1 - \beta)} \int_0^x \frac{u'(\xi)d\xi}{(x-x)^\beta}, \quad (2.29)$$

$$xD^\beta_L u(x) = \frac{u(L)(L-x)^{-\beta}}{\Gamma(1 - \beta)} + \frac{1}{\Gamma(1 - \beta)} \int_x^L \frac{u'(\xi)d\xi}{(x-x)^\beta}. \quad (2.30)$$

Using the link between the Riemann-Liouville and Grünwald-Letnikov fractional derivatives [116], the second term of the right-hand side of Eq. (2.29) can be approximated at $x = x_l$ by

$$\frac{1}{\Gamma(1 - \beta)} \int_0^{x_l} \frac{u'(\xi)d\xi}{(x_l - \xi)^\beta} = \frac{1}{\Gamma(1 - \beta)} \int_0^{x_l} \frac{u'(x_l - \xi)d\xi}{\xi^\beta}$$
$$= \frac{1}{\Gamma(1 - \beta)} \sum_{j=0}^{l-1} \int_{j h}^{(j+1)h} \frac{u'(x_l - \xi)d\xi}{\xi^\beta}$$
$$\approx \frac{1}{\Gamma(1 - \beta)} \sum_{j=0}^{l-1} \frac{u(x_l - j h) - u(x_l - (j+1)h)}{h} \int_{j h}^{(j+1)h} \frac{d\xi}{\xi^\beta}$$
$$= \frac{h^{-\beta}}{\Gamma(2 - \beta)} \sum_{j=0}^{l-1} (u_{l-j} - u_{l-j-1})[(j+1)^{1-\beta} - j^{1-\beta}],$$

where $u(x_l - j h) = u_{l-j}$.

Hence, we obtain an approximation of the left-handed fractional derivative (2.29) with $0 < \beta < 1$ as

$$0D^\beta_x u(x_l) \approx \frac{h^{-\beta}}{\Gamma(2 - \beta)} \left\{ \frac{(1 - \beta)u_0}{l^\beta} + \sum_{j=0}^{l-1} (u_{l-j} - u_{l-j-1})[(j+1)^{1-\beta} - j^{1-\beta}] \right\}. \quad (2.31)$$

Similarly, we can derive an approximation of the right-handed fractional derivative (2.30) with
0 < \beta < 1 as

\[ x D_L^\beta u(x_l) \approx \frac{h^{-\beta}}{\Gamma(2 - \beta)} \left\{ \frac{(1 - \beta) u_N}{(N - l)^\beta} + \sum_{j=0}^{N-l-1} (u_{l+j} - u_{l+j+1})[(j + 1)^{1-\beta} - j^{1-\beta}] \right\}. \]

(2.32)

Using the numerical approximations (2.31) and (2.32), the advection term of the RFADE (2.25) can be approximated by

\[ K_\beta \partial_{|x|^\beta}^\beta u(x_l) \approx -\frac{K_\beta h^{-\beta}}{2 \cos(\frac{\pi \beta}{2}) \Gamma(2 - \beta)} \left\{ \frac{(1 - \beta) u_0}{l^\alpha} + \frac{(2 - \alpha)}{l^{a-1}}(u_1 - u_0) \right. \\
+ \sum_{j=0}^{l-1} (u_{l-j} - 2u_{l-j} + u_{l-j-1})[(j + 1)^{2-\alpha} - j^{2-\alpha}] \\
+ \frac{(1 - \alpha)(2 - \alpha) u_N}{(N - l)^\alpha} + \frac{(2 - \alpha)}{(N - l)^{(a-1)}}(u_N - u_{N-1}) \\
+ \sum_{j=0}^{N-l-1} (u_{l+j+1} - 2u_{l+j} + u_{l+j+1})[(j + 1)^{2-\alpha} - j^{2-\alpha}] \right\}. \]

(2.33)

Therefore, using the numerical approximation of the diffusion term (2.16) and the numerical approximation of the advection term (2.33), we transform the RFADE (2.25) based on Definition 2.1 and Lemma 2.1 into the following system of TODEs

\[
\frac{du_l}{dt} \approx -\frac{K_\alpha h^{-\alpha}}{2 \cos(\frac{\pi \alpha}{2}) \Gamma(3 - \alpha)} \left\{ \frac{(1 - \alpha)(2 - \alpha) u_0}{l^{\alpha}} + \frac{(2 - \alpha)}{l^{\alpha-1}}(u_1 - u_0) \right. \\
+ \sum_{j=0}^{l-1} (u_{l-j+1} - 2u_{l-j} + u_{l-j-1})[(j + 1)^{2-\alpha} - j^{2-\alpha}] \\
+ \frac{(1 - \alpha)(2 - \alpha) u_N}{(N - l)^\alpha} + \frac{(2 - \alpha)}{(N - l)^{(a-1)}}(u_N - u_{N-1}) \\
+ \sum_{j=0}^{N-l-1} (u_{l+j+1} - 2u_{l+j} + u_{l+j+1})[(j + 1)^{2-\alpha} - j^{2-\alpha}] \right\} \\
- \frac{K_\beta h^{-\beta}}{2 \cos(\frac{\pi \beta}{2}) \Gamma(2 - \beta)} \left\{ \frac{(1 - \beta) u_0}{l^\beta} + \frac{(1 - \beta)}{(N - l)^\beta}(u_N - u_{N-1}) \right. \\
+ \sum_{j=0}^{l-1} (u_{l-j} - 2u_{l-j} + u_{l-j-1})[(j + 1)^{1-\beta} - j^{1-\beta}] + \frac{(1 - \beta) u_N}{(N - l)^\beta} \\
+ \sum_{j=0}^{N-l-1} (u_{l+j+1} - 2u_{l+j} + u_{l+j+1})[(j + 1)^{1-\beta} - j^{1-\beta}] \right\}. \]

(2.34)

where \( l = 1, \ldots, N - 1 \). This system of TODEs is then solved using the standard ODE solver, DASSL.
2.4.3 Shifted and standard Grünwald approximation method for the RFADE

In this subsection, we present a shifted and standard Grünwald approximation method for the RFADE (2.25) based on Definition 2.1 and Lemma 2.1. Note that approximating both the diffusion and advection terms by either the shifted Grünwald method or by the standard Grünwald method results in an unstable scheme. Hence, the diffusion term is approximated by the shifted Grünwald method as presented in Section 2.3.3, and the advection term is approximated by the standard Grünwald formulae [116] as follows:

\[ 0D^\beta_x u(x_l) = \frac{1}{h^\beta} \sum_{j=0}^l w_j u_{l-j} + O(h), \quad xD^\beta_L u(x_l) = \frac{1}{h^\beta} \sum_{j=0}^{N-l} w_j u_{l+j} + O(h), \]

where the coefficients are defined by

\[ w_0 = 1, \quad w_j = (-1)^j \frac{\beta(\beta - 1) \cdots (\beta - j + 1)}{j!}, \]

for \( j = 1, 2, \ldots, N \).

Then, the RFADE (2.25) based on Definition 2.1 and Lemma 2.1 can be cast into the following system of TODEs:

\[
\frac{du_l}{dt} \approx -\frac{K_\alpha}{2 \cos(\frac{\pi \alpha}{2}) h^\alpha} \left[ \sum_{j=0}^{l+1} g_j u_{l-j+1} + \sum_{j=0}^{N-l+1} g_j u_{l+j-1} \right] \\
- \frac{K_\beta}{2 \cos(\frac{\pi \beta}{2}) h^\beta} \left[ \sum_{j=0}^{l} w_j u_{l-j} + \sum_{j=0}^{N-l} w_j u_{l+j} \right],
\]

(2.35)

which can again be solved using DASSL.

2.4.4 Matrix transform method for the RFADE

The matrix transform technique presented in Section 2.3.4 can be easily applied to the advection term \(-K_\beta (-\Delta)^{\frac{\beta}{2}} u(x, t), (0 < \beta < 1)\). Hence, we obtain the matrix representation for
2.5 Numerical results for the RFDE and RFADE

In this section, we provide numerical examples for the RFDE and RFADE to demonstrate the effectiveness of these numerical methods. We also use our solution methods to demonstrate the changes in solution behaviour that arise when the exponent is varied from integer order to fractional order, and to identify the differences between solutions with and without the advection term.

2.5.1 Numerical examples of the RFDE

In this subsection, we present two examples of the RFDE on a finite domain.

Example 2.1. We consider the following RFDE:

\[
\frac{\partial u(x,t)}{\partial t} = -K_\alpha \frac{\partial^{\alpha}}{\partial |x|^\alpha} u(x,t), \quad 0 < t \leq T, \quad 0 < x < \pi, \quad 1 < \alpha \leq 2, \quad (2.36)
\]

\[
u(x,0) = x^2(\pi - x), \quad (2.37)
\]

\[
u(0,t) = u(\pi,t) = 0. \quad (2.38)
\]

According to Section 2.3.1, the analytic solution of Eq.(2.36)-(2.38) based on Definition 2.2 is given by

\[
u(x,t) = \sum_{n=1}^{\infty} b_n \sin(nx) \exp(-n^2) K_\alpha t. \quad (2.38)
\]
where

\[ b_n = c_n(0) = \frac{2}{\pi} \int_0^{\pi} g(\xi) \sin\left(\frac{n\pi \xi}{\pi}\right) d\xi = \frac{2}{\pi} \int_0^{\pi} \xi^2 (\pi - \xi) \sin(n\xi) d\xi = \frac{8}{n^3} (-1)^{n+1} - \frac{4}{n^3}. \]

Figure 2.1: Comparison of the numerical solutions with the analytic solution at \( t = 0.4 \) for the RFDE (2.36)-(2.38) with \( K_\alpha = 0.25 \) and \( \alpha = 1.8 \).

Figure 2.1 shows the analytic solution and the solutions obtained by the three numerical methods proposed in Sections 2.3.2-2.3.4, for \( t = 0.4, \alpha = 1.8 \) and \( K_\alpha = 0.25 \). From Figure 2.1, it can be seen that all three numerical solutions are in good agreement with the analytic solution. Since both the MTM and analytic solution are based on Definition 2.2, we only present here the maximum errors of the MTM in Table 2.1. From Table 2.1, it can be seen that the MTM is stable and convergent for solving the RFDE (2.36)-(2.38) based on Definition 2.2. The solution profiles of the RFDE for different values of \( \alpha = 1.2, 1.4, 1.6, 1.8, 2.0 \) when \( t = 0.5, 1.5, 2.5, 3.5 \) are shown in Figure 2.2. It can be seen that the process described by the RFDE is slightly more skewed to the right than that modelled by the standard diffusion equation.

To further demonstrate the impact of fractional order to the solution behaviour, another example of the RFDE with a different initial condition is now considered.
Table 2.1: Maximum errors of the MTM for solving the RFDE (2.36)-(2.38)

<table>
<thead>
<tr>
<th>$h = \pi/N$</th>
<th>MTM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi/10$</td>
<td>2.217E-2</td>
</tr>
<tr>
<td>$\pi/20$</td>
<td>5.759E-3</td>
</tr>
<tr>
<td>$\pi/40$</td>
<td>1.481E-3</td>
</tr>
<tr>
<td>$\pi/80$</td>
<td>3.727E-4</td>
</tr>
</tbody>
</table>

Figure 2.2: The numerical approximation of $u(x, t)$ for the RFDE (2.36)-(2.38) with different values of $\alpha = 1.2, 1.4, 1.6, 1.8, 2.0$ when $t = 0.5, 1.5, 2.5, 3.5$. 
Example 2.2. We consider the following RFDE:

\[
\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t), \quad 0 < t \leq T, \quad 0 < x < \pi, \quad 1 < \alpha \leq 2 \tag{2.39}
\]

\[
u(x,0) = \sin 4x, \quad \tag{2.40}
\]

\[
u(0,t) = u(\pi,t) = 0. \quad \tag{2.41}
\]

Figure 2.3 presents the solution profiles of the RFDE (2.39)-(2.41) over space for \(1 < \alpha \leq 2\) when \(t = 0.5\). It can be observed that as \(\alpha\) is decreased from 2 to 1 the amplitude of the sinusoidal solution behaviour is increased. Figure 2.4 displays the solution profiles of the RFDE (2.39)-(2.41) over space for \(0 < t < 1\) when \(\alpha = 2.0\) (left) and \(\alpha = 1.5\) (right), respectively. We can see that the fractional diffusion \((\alpha = 1.5)\) is slower than the standard diffusion \((\alpha = 2.0)\). From Figures 2.1-2.4, we conclude that the solution continuously depends on the Riesz space fractional derivatives.

![Graph of u(x,t) for the RFDE (2.39)-(2.41)](image)

Figure 2.3: The numerical approximation of \(u(x,t)\) for the RFDE (2.39)-(2.41) when \(t = 0.5\) and \(K_\alpha = 0.25\).

2.5.2 Numerical examples of the RFADE

In this subsection, we present three examples of the RFADE on a finite domain.
2.5 Numerical results for the RFDE and RFADE

Figure 2.4: A comparison of solutions for the RFDE (2.39)-(2.41) with $K_\alpha = 0.25$ when $\alpha = 2$ (left) and $\alpha = 1.5$ (right).

Example 2.3. We consider the following RFADE:

\[
\frac{\partial u(x,t)}{\partial t} = -K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) - K_\beta \frac{\partial^\beta}{\partial |x|^\beta} u(x,t), \quad 0 < x < \pi, \quad (2.42)
\]

\[
u(x,0) = x^2(\pi - x), \quad (2.43)
\]

\[
u(0,t) = \nu(\pi,t) = 0. \quad (2.44)
\]

According to Section 2.4.1, the analytic solution of Eq.(2.42)-(2.44) based on Definition 2.2 is given by

\[
u(x,t) = \sum_{n=1}^{\infty} \left[ \frac{8}{n^3} (-1)^{n+1} - \frac{4}{n^3} \right] \sin(nx) \exp(-[K_\alpha (n^\alpha)^{\frac{\alpha}{2}} + K_\beta (n^\beta)^{\frac{\beta}{2}}]t). \quad (2.45)
\]

Figure 2.5 shows the analytic solution and the solutions obtained by the three numerical methods proposed in Sections 2.4.2-2.4.4, for $t = 0.4$, $\alpha = 1.8$, $\beta = 0.4$, and $K_\alpha = K_\beta = 0.25$. From Figure 2.5, it can be seen that all three numerical methods are again in good agreement with the analytic solution. From Table 2.2, it can be seen that the MTM is stable and convergent for solving the RFADE (2.42)-(2.44) based on Definition 2.2.

Figure 2.6 shows the solution profiles for different values of $\alpha$ at different times $t$, while Figure
Figure 2.5: Comparison of the numerical solutions with the analytic solution at $t = 0.4$ for the RFAD (2.42)-(2.44) with $\alpha = 1.8$, $\beta = 0.4$, and $K_\alpha = K_\beta = 0.25$.

<table>
<thead>
<tr>
<th>$h = \pi/N$</th>
<th>MTM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\pi/10$</td>
<td>1.9963E-2</td>
</tr>
<tr>
<td>$\pi/20$</td>
<td>5.1683E-3</td>
</tr>
<tr>
<td>$\pi/40$</td>
<td>1.3386E-3</td>
</tr>
<tr>
<td>$\pi/80$</td>
<td>3.3519E-4</td>
</tr>
</tbody>
</table>

Table 2.2: Maximum errors of the MTM for solving the RFAD (2.42)-(2.44)

2.7 shows the solution profiles for different values of $\beta$ at different times $t$. In both figures, it can be seen that the process described by the RFAD is again slightly more skewed to the right than that modelled by the classical ADE ($\alpha = 2$, $\beta = 1$).

In order to demonstrate the convergence of both the L1/L2 approximation method and the standard/shifted Grünwald approximation method, we consider another example of the RFAD based on Definition 2.1 and Lemma 2.1.

**Example 2.4.** We now consider the following RFAD with a source term

\[
\frac{\partial u(x, t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x, t) + K_\beta \frac{\partial^\beta}{\partial |x|^\beta} u(x, t) + f(x, t), \quad 0 < x < 1, \quad (2.46)
\]

\[
u(x, 0) = 0, \quad (2.47)
\]

\[
u(0, t) = u(1, t) = 0, \quad (2.48)
\]
2.5 Numerical results for the RFDE and RFADE

Figure 2.6: The numerical approximation of $u(x, t)$ for the RFADE (2.42)-(2.44) with different values of $\alpha = 1.2, 1.4, 1.6, 1.8, 2.0$ when $\beta = 0.4$ and $t = 0.5, 1.5, 2.5, 3.5$.

where

$$f(x, t) = \frac{K_\alpha t^\alpha e^{\beta t}}{2 \cos(\alpha \pi/2)} \left\{ \frac{2}{\Gamma(3 - \alpha)} \left[ x^{2-\alpha} + (1 - x)^{2-\alpha} \right] 
- \frac{12}{\Gamma(4 - \alpha)} \left[ x^{3-\alpha} + (1 - x)^{3-\alpha} \right] + \frac{24}{\Gamma(5 - \alpha)} \left[ x^{4-\alpha} + (1 - x)^{4-\alpha} \right] \right\} 
+ \frac{K_\beta t^\alpha e^{\beta t}}{2 \cos(\beta \pi/2)} \left\{ \frac{2}{\Gamma(3 - \beta)} \left[ x^{2-\beta} + (1 - x)^{2-\beta} \right] 
- \frac{12}{\Gamma(4 - \beta)} \left[ x^{3-\beta} + (1 - x)^{3-\beta} \right] + \frac{24}{\Gamma(5 - \beta)} \left[ x^{4-\beta} + (1 - x)^{4-\beta} \right] \right\} 
+ t^{\alpha-1} e^{\beta t} (\alpha + \beta t)x^2(1 - x)^2. \tag{2.49}$$

The exact solution of Eq.(2.46)-(2.48) based on Definition 2.1 and Lemma 2.1 is given by

$$u(x, t) = t^\alpha e^{\beta t} x^2(1 - x)^2.$$

In this example, we take $\alpha = 1.7$, $\beta = 0.4$, $K_\alpha = K_\beta = 2.0$, $t = 2.0$. Table 2.3 shows the convergence of both the L1/L2 approximation method and the standard/shifted Grünwald approximation method for solving the RFADE (2.46)-(2.48) based on Definition 2.1 and Lemma 2.1. From Table 2.3, it can be seen that both methods are stable and convergent.

To further demonstrate the impact of fractional order, another example of the RFADE with a
Figure 2.7: The numerical approximation of \( u(x, t) \) for the RFADE (2.42)-(2.44) with different values of \( \beta = 0.1, 0.3, 0.5, 0.9 \) when \( \alpha = 1.8 \) and \( t = 0.5, 1.5, 2.5, 3.5 \).

Table 2.3: Maximum errors of the \( L1/L2 \) approximation method and the standard/shifted Grünwald method for solving the RFADE (2.46)-(2.48)

<table>
<thead>
<tr>
<th>( h = 1/N )</th>
<th>( L1/L2 )</th>
<th>Standard/Shifted Grünwald</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/50</td>
<td>1.8144E-2</td>
<td>2.8191E-3</td>
</tr>
<tr>
<td>1/100</td>
<td>9.4917E-3</td>
<td>1.5093E-3</td>
</tr>
<tr>
<td>1/200</td>
<td>4.8584E-3</td>
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<tr>
<td>1/400</td>
<td>2.4586E-3</td>
<td>3.9459E-4</td>
</tr>
</tbody>
</table>

different initial condition is now considered.

Example 2.5.

\[
\frac{\partial u(x, t)}{\partial t} = K_\alpha \frac{\partial^\alpha u(x, t)}{\partial|x|^\alpha} + K_\beta \frac{\partial^\beta u(x, t)}{\partial|x|^\beta}, \quad 0 < x < \pi, \quad t > 0, \quad (2.50)
\]

\[
u(x, 0) = \sin 4x, \tag{2.51}
\]

\[
u(0, t) = u(\pi, t) = 0. \tag{2.52}
\]

Figures 2.8 and 2.9 displays the changes in the solution behaviours when \( \alpha \) varies from 1 to 2 and \( \beta \) ranges from 0 to 1, respectively. In both figures, consistent with our observations for the RFDE (2.39)-(2.41) in Section 2.5.1, we see that as \( \alpha \) is decreased from 2 to 1 or \( \beta \) from 1 to 0 the amplitude of the sinusoidal solution behaviour is increased. In Figure 2.10, the solution profiles of RFADE over space for \( 0 < t < 1 \) are displayed when \( \alpha = 2.0, \beta = 1.0 \) (left)
and $\alpha = 1.5$, $\beta = 0.7$ (right), respectively. It can be observed that the fractional advection-dispersion process ($\alpha = 1.5$, $\beta = 0.7$) is slower than the classical advection-dispersion process ($\alpha = 2.0$, $\beta = 1.0$). Furthermore, from Figures 2.8-2.10, it is seen that the solution continuously depends on the Riesz space fractional derivatives. Finally, Figure 2.11 provides a comparison of the RFDE (2.39)-(2.41) and RFADE (2.50)-(2.52) with $K_\alpha = K_\beta = 0.25$ at time $t = 0.5$, where it can be observed that there is an offset when the fractional advection term is added to the fractional diffusion process.

Figure 2.8: The numerical approximation of $u(x, t)$ for the RFADE (2.50)-(2.52) when $\beta = 0.7$ and $t = 0.5$.

### 2.6 Conclusions

In this paper, three effective numerical methods for solving the RFDE and RFADE on a finite domain with homogeneous Dirichlet boundary conditions have been described. Two existing definitions of the operator $-(-\Delta)^{\beta/2}$ are investigated and discussed. Numerical results have demonstrated the effectiveness and convergence of the three numerical methods. The methods and techniques discussed in this paper can also be applied to solve other kinds of fractional partial differential equations, e.g., the modified fractional diffusion equation where $1 < \beta < \alpha \leq 2$. 
Figure 2.9: The numerical approximation of $u(x, t)$ for the RFADE (2.50)-(2.52) when $\alpha = 1.5$ and $t = 0.5$.

Figure 2.10: A comparison of solutions for the RFADE (2.50)-(2.52) when $\alpha = 2.0$ and $\beta = 1.0$ (left) and $\alpha = 1.5$ and $\beta = 0.7$ (right).
2.6 Conclusions

Figure 2.11: Comparison of the RFDE (2.39)-(2.41) and RFADE (2.50)-(2.52) with $K_{\alpha} = K_{\beta} = 0.25$ at time $t = 0.5$. 
3.1 Introduction

A growing number of works in science and engineering deal with dynamical systems described by fractional order equations that involve derivatives and integrals of non-integer order \[ [13, 55, 110, 160] \]. These new models are more adequate than the previously used integer order models, because fractional order derivatives and integrals enable the description of the memory and hereditary properties of different substances \[ [116] \]. This is the most significant advantage of the fractional order models in comparison with integer order models, in which such effects are neglected. In the context of flow in porous media, fractional space derivatives model large motions through highly conductive layers or fractures, while fractional time derivatives describe particles that remain motionless for extended periods of time \[ [103] \].

In this paper, we consider the following time and space-symmetric fractional diffusion equation
Chapter 3. Analytical and numerical solutions for TSS-FDE

(TSS-FDE):

\[ t^\alpha D^\alpha u(x,t) = -K_\beta (-\Delta)^{\beta/2} u(x,t), \quad 0 \leq t \leq T, \quad 0 \leq x \leq L, \quad (3.1) \]

subject to either homogeneous Dirichlet boundary conditions, or homogeneous Neumann boundary conditions

\[ u(0, t) = u(L, t) = 0, \quad \text{or} \quad \frac{\partial u}{\partial x}(0, t) = \frac{\partial u}{\partial x}(L, t) = 0, \quad (3.2) \]

and the initial condition

\[ u(x, 0) = g(x), \quad (3.3) \]

where \( u \) is a solute concentration and \( K_\beta \) represents the dispersion coefficient. \( t^\alpha D^\alpha \) is the Caputo time fractional derivative of order \( \alpha \) \((0 < \alpha < 1)\) with starting point at \( t = 0 \) defined as follows [116]:

\[ t^\alpha D^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{\partial u(x,\eta)}{\partial \eta} \frac{d\eta}{(t-\eta)\alpha}. \quad (3.4) \]

The symmetric space fractional derivative \(-(-\Delta)^{\beta/2}\) of order \( \beta \) \((1 < \beta \leq 2)\) is defined by Gorenflo and Mainardi [48], where \( \Delta \) is the Laplacian operator.

Physical considerations of a fractional diffusion equation restrict \( 0 < \alpha < 1, 1 < \beta \leq 2 \), and we assume \( K_\beta > 0 \) so that the flow is from left to right. The physical meaning of using homogeneous Dirichlet boundary conditions is that the boundary is set far enough away from an evolving plume such that no significant concentrations reach that boundary [105, 107].

Also, by assuming homogeneous Dirichlet boundary conditions, we derive that the Riesz fractional derivative is equivalent to the fractional power of Laplacian operator [150], that is, \( \partial^\beta u(x,t)/\partial|x|^\beta = -(-\Delta)^{\beta/2} u(x,t) \). The physical meaning of using homogeneous Neumann boundary conditions is that the tracer moves freely through the boundaries [106].

In the case of \( \alpha = 1, \beta = 2 \), the TSS-FDE \((3.1)\) reduces to the classical diffusion equation.

For \( 0 < \alpha < 1, \beta = 2 \), the TSS-FDE \((3.1)\) models subdiffusion due to particles having heavy-tailed resting times, while for \( \alpha = 1, 1 < \beta < 2 \) it corresponds to the Lévy process [160].
3.2 Analytical solutions

Hence, the solution of TSS-FDE (3.1) is important for describing the competition between these two anomalous diffusion processes. The TSS-FDE was first introduced by Zaslavsky [161] to model Hamiltonian chaos. More recently, an important application of TSS-FDE arises in finance [104], where coupled continuous time random walk (CTRW) models were used to describe the movement of log-prices. In these coupled CTRW models, the probability density functions for the limiting stochastic process solve TSS-FDE.

3.2 Analytical solutions

In this section, using the method of separation of variables, the analytical solution of TSS-FDE (3.1)–(3.3) is first derived under homogeneous Dirichlet boundary conditions. For homogeneous Neumann conditions, a similar method can be used to derive the analytical solution.

Setting $u(x, t) = X(x)T(t)$ and substituting into (3.1) yields

\[ t D_\alpha X(x)T(t) + K_\beta (-\Delta)^{\beta/2} X(x)T(t) = 0. \]

Letting $-\omega$ be the separation constant we obtain two fractional ordinary linear differential equations for $X(x)$ and $T(t)$, respectively as

\[ (-\Delta)^{\beta/2} X(x) - \omega X(x) = 0, \quad (3.5) \]
\[ t D_\alpha X(t) + K_\beta \omega T(t) = 0. \quad (3.6) \]

Following the definition given by Ilić et al. [61] of the fractional Laplacian $(-\Delta)^{\beta/2}$ defined on a bounded region, (3.5) can be expressed as

\[ \sum_{n=1}^{\infty} c_n (\lambda_n^2)^{\beta/2} x_n + \omega_n \sum_{n=1}^{\infty} c_n x_n = 0. \quad (3.7) \]

Hence, under homogeneous Dirichlet conditions, the eigenvalues of (3.5) are $\omega_n = \lambda_n^{\beta} = (n\pi/L)^\beta$ for $n = 1, 2, \ldots$, and the corresponding eigenfunctions are nonzero constant multiples of $x_n = \sin(n\pi x/L)$. For homogeneous Neumann conditions, the eigenvalues are $\omega_n = \lambda_n^{\beta} = (n\pi/L)^\beta$ for $n = 0, 1, 2, \ldots$, and the corresponding eigenfunctions are $x_n = \cos(n\pi x/L)$. 
Next, we seek a solution of the TSS-FDE (3.1) under homogeneous Dirichlet conditions in the form

\[ u(x, t) = \sum_{n=1}^{\infty} T_n(t) \sin \left( \frac{n\pi x}{L} \right). \]  
(3.8)

Substituting (3.8) into (3.1) yields

\[ tD_\alpha^\ast T_n(t) = -K_\beta \omega_n T_n(t). \]  
(3.9)

Since \( u(x, t) \) must also satisfy the initial conditions (3.3)

\[ \sum_{n=1}^{\infty} T_n(0) \sin \left( \frac{n\pi x}{L} \right) = g(x), \quad 0 \leq x \leq L, \]  
(3.10)

and therefore

\[ T_n(0) = \frac{2}{L} \int_{0}^{L} g(x) \sin \left( \frac{n\pi x}{L} \right) dx, \quad n = 1, 2, \ldots. \]  
(3.11)

For each value of \( n \), (3.9) and (3.11) compose a fractional initial value problem. Applying the Laplace transform to (3.9), we obtain

\[ \tilde{T}_n(s) = \frac{s^{\alpha-1}T_n(0)}{s^\alpha + K_\beta \omega_n}. \]  
(3.12)

By using the known inverse Laplace transform [129]

\[ E_\alpha(-\omega t^\alpha) = \mathcal{L}^{-1} \left\{ \frac{s^{\alpha-1}}{s^\alpha + \omega} \right\}, \quad \Re(s) > |\omega|^{1/\alpha}, \]  
(3.13)

we obtain the analytical solution of TSS-FDE (3.1) under homogeneous Dirichlet conditions as

\[ u(x, t) = \sum_{n=1}^{\infty} T_n(t) \sin \left( \frac{n\pi x}{L} \right) = \sum_{n=1}^{\infty} E_\alpha(-K_\beta \omega_n t^\alpha)T_n(0) \sin \left( \frac{n\pi x}{L} \right), \]  
(3.14)

where \( T_n(0) \) is given in (3.11), and \( E_\alpha(z) \) is the Mittag–Leffler function [116]

\[ E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(an + 1)}, \quad \alpha > 0. \]  
(3.15)
3.3 Numerical methods

Here, when $\alpha = 1$, the solution (3.14) corresponds precisely with the results derived for the Riesz space fractional diffusion equation [150].

Similarly, the analytical solution of TSS-FDE (3.1) under homogeneous Neumann conditions is

$$
u(x,t) = \sum_{n=0}^{\infty} T_n(t) \cos \left( \frac{n\pi x}{L} \right)
= \frac{1}{2} T_0(0) + \sum_{n=1}^{\infty} E_\alpha(-K_\beta \omega_n t^\alpha) T_n(0) \cos \left( \frac{n\pi x}{L} \right),
$$

(3.16)

where $T_n(0) = \frac{2}{L} \int_0^L g(x) \cos(n\pi x/L) dx$, $n = 0, 1, 2, \ldots$, and we have used the result that $E_\alpha(0) = 1$.

### 3.3 Numerical methods

In this section, we present two numerical schemes to simulate the solution behaviour of TSS-FDE (3.1)–(3.3). In Section 3.3.1, a finite difference method (FDM) and the matrix transform method (MTM) are used to discretise the Caputo time fractional derivative and the symmetric space fractional derivative, respectively. In Section 3.3.2, using the Laplace transform method (LTM) together with the MTM, we transfer the TSS-FDE (3.1) into a discrete system describing the evolution of $u(x,t)$ in space and time.

Using time stepping methods in the fractional case requires the storage of all previous time steps. The difficulty in solving fractional differential equations, particularly where the application area requires a solution to be given over a long time interval, is essentially because fractional derivatives are non-local operators. The so-called non-local property means that the next state of a system not only depends on its current state, but also on the historical states starting from the initial time. This property is closer to reality and is the main reason why fractional calculus has become more and more useful. To overcome this difficulty, some authors explore techniques for reducing computational cost that keeps the error under control. The simplest approach is to disregard the tail of the integral and to integrate only over a fixed period of recent history. This is commonly referred to as the 'short-memory' principle, and is described by Podlubny [116]. Here, we only consider the full memory case.
3.3.1 Finite difference method with matrix transform method

Let \( x_l := lh, l = 0, 1, \ldots, M \), where \( h := L/M \) is the space step; \( t_n := n\tau, n = 0, 1, \ldots, N \), where \( \tau := T/N \) is the time step; and \( u^n_l \) denote the numerical approximation of \( u(x_l, t_n) \).

Adopting the FDM given by Lin & Xu [76], we discretise the Caputo time fractional derivative as

\[
 t^\alpha D^\ast u^{n+1}_l = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^{n} b_j [u^{n+1-j}_l - u^{n-j}_l] + O(\tau^{2-\alpha}),
\]

written in matrix form

\[
 t^\alpha D^\ast U^{n+1} = \frac{1}{\mu_0} \sum_{j=0}^{n} b_j [U^{n+1-j} - U^{n-j}] + O(\tau^{2-\alpha}),
\]

where \( \mu_0 = \tau^\alpha \Gamma(2-\alpha) \), \( b_j = (j+1)\Gamma(1-\alpha) - j\Gamma(1-\alpha), j = 0, 1, 2, \ldots, n \).

Utilising the theory described by Ilić et al. [61], we find a matrix representation of the fractional Laplacian operator

\[
 -(-\Delta)^{\beta/2} U \approx -\frac{1}{h^\beta} A^{\beta/2} U,
\]

where \( A = \text{tridiag}(-1, 2, -1) \in \mathbb{R}^{(M-1)\times(M-1)} \) under homogeneous Dirichlet conditions, or

\[
 A = \begin{bmatrix}
 1 & -1 & \quad & \quad & \quad \\
 -1 & 2 & -1 & \quad & \quad \\
 \quad & \ddots & \ddots & \ddots & \quad \\
 \quad & -1 & 2 & -1 & \quad \\
 \quad & \quad & -1 & 1 & \quad \\
 \end{bmatrix}_{(M+1)\times(M+1)},
\]

under homogeneous Neumann conditions. Since the matrix \( A \) is symmetric positive definite (SPD), there exits a nonsingular matrix \( P \) that orthogonally diagonalises \( A \) as

\[
 A = P \Lambda P^T,
\]

where \( \Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{M-1}) \) under homogeneous Dirichlet conditions or \( \Lambda = \text{diag}(\lambda_0, \lambda_1, \ldots, \lambda_M) \) under homogeneous Neumann conditions, \( \lambda_i(i = 0, 1, 2, \ldots, M) \).
being the eigenvalues of $A$. Thus, the fractional Laplacian can be expressed in terms of its spectral decomposition as
\[-(-\Delta)^{\beta/2}U \approx -\frac{1}{h^\beta}P\Lambda^{\beta/2}P^TU.\] (3.21)

Now, combining (3.18) with (3.21), we obtain the following numerical difference approximation of the TSS-FDE (3.1):
\[
\frac{1}{\mu_0} \sum_{j=0}^{n} b_j[U^{n+1-j} - U^{n-j}] = -\eta_\beta P\Lambda^{\beta/2}P^TU^{n+1},
\] (3.22)
where $\eta_\beta = K_\beta/h^\beta$. After simplification,
\[
\left[ b_0I + \mu_0\eta_\beta P\Lambda^{\beta/2}P^T \right] U^{n+1} = \sum_{j=0}^{n-1} (b_j - b_{j+1})U^{n-j} + b_nU^0,
\] (3.23)
where $U^0$ is the matrix representation of the initial value $g(x)$.

### 3.3.2 Laplace transform method with matrix transform method

We now consider an alternative strategy for approximating the fractional ODE system associated with the TSS-FDE (3.1), when the approximation for the fractional Laplacian is given by (3.19):
\[
iD_\alpha^n U^n = -\eta_\beta A^{\beta/2}U^n.
\] (3.24)

Applying the Laplace transform to (3.24) with $\tilde{U}^n = \mathcal{L}\{U^n(t)\}$ yields
\[
\tilde{U}^n = \left[ sI + s^{1-\alpha}\eta_\beta A^{\beta/2} \right]^{-1} U^0.
\] (3.25)

Since $A$ is SPD and has the orthogonal diagonalisation (3.20), we obtain
\[
U^n = P\mathcal{L}^{-1}\left\{ \left( sI + s^{1-\alpha}\eta_\beta A^{\beta/2} \right)^{-1} \right\} P^TU^0.
\] (3.26)

Recalling (3.13) and applying the inverse Laplace transform for each of the eigenvalues, we
obtain the second numerical scheme for approximating the TSS-FDE (3.1) as

\[ U^n = PE_\alpha\left(-t^n_\eta\Lambda^{\beta/2}\right)P^T U^0, \tag{3.27} \]

where \( E_\alpha(z) \) is the Mittag–Leffler function defined in (3.15).

### 3.4 Numerical examples

In this section, we provide two examples of the TSS-FDE to assess the accuracy of the two numerical schemes proposed in Section 3.3, and to illustrate the solution behaviour that arises as we change from integer to fractional order in time and space.

**Example 3.1.** Considering the following TSS-FDE with homogeneous Neumann boundary conditions:

\[ \substack{\mathcal{D}_x^\alpha u(x,t) = -(-\Delta)^{\beta/2}u(x,t), \quad 0 \leq t \leq T,
\quad 0 \leq x \leq \pi, \\
\frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(L,t) = 0, \\
u(x,0) = x^2\left(\frac{3}{2}\pi - x\right).} \tag{3.28-3.30} \]

Following the solution method (3.16) derived in Section 3.2, the analytical solution of TSS-FDE (3.28)–(3.30) is

\[ u(x,t) = \frac{\pi^3}{4} + \sum_{n=1}^{\infty} \frac{12[(-1)^n - 1]}{\pi n^4} E_\alpha(-n^{\beta}t^{\alpha}) \cos(nx). \tag{3.31} \]

Figure 3.1(a) shows that both numerical solution schemes provide a good match with the analytical solution (3.31) at different times \( t \), with \( \alpha = 0.5, \beta = 1.5, M = 50, N = 100. \)

**Example 3.2.** Consider the following TSS-FDE with homogeneous Dirichlet boundary conditions:

\[ \substack{\mathcal{D}_x^\alpha u(x,t) = -(-\Delta)^{\beta/2}u(x,t), \quad 0 \leq t \leq T,
\quad 0 \leq x \leq \pi, \\
u(0,t) = u(\pi,t) = 0, \\
u(x,0) = x^2(\pi - x).} \tag{3.32-3.34} \]
3.4 Numerical examples

Figure 3.1: Comparison of the numerical solutions with the exact solution at different times \( t = 0.1, 1.0, 5.0 \) for (a) the TSS-FDE \((3.28)-(3.30)\), and (b) the TSS-FDE \((3.32)-(3.34)\), with \( \alpha = 0.5, \beta = 1.5, M = 50, N = 100 \).

According to \((3.14)\), the exact solution of TSS-FDE \((3.32)-(3.34)\) is

\[
 u(x, t) = \sum_{n=1}^{\infty} \frac{8(-1)^{n+1}}{n^\beta} E_\alpha(\frac{-n^\beta t^\alpha}{2}) \sin(nx). \tag{3.35}
\]

Figure 3.1(b) shows that both numerical solution schemes provide a good match with the analytical solution \((3.35)\) at different times \( t \), with \( \alpha = 0.5, \beta = 1.5, M = 50, N = 100 \). Furthermore, in Tables 3.1 and 3.2, we see that the maximum errors are decreasing as the spatial and temporal nodes increase. Especially, the LTM-MTM is more accurate than the FDM-MTM because it is exact in time. The error observed in the tables for the LTM-MTM is only associated with the spatial discretisation error. More rigorous analyses on stability and convergence will be investigated in future work.

Figure 3.2(a) displays the solution profiles of the TSS-FDE \((3.32)-(3.34)\) over space for \( 0 < \alpha < 1, \beta = 1.5 \) at \( t = 1.0 \). As \( \alpha \) is increased over the interval \((0, 1)\) the solution profile diminishes in magnitude and becomes slightly more skewed. The solution profiles for selected values of \( \beta \) with \( \alpha = 0.5 \) at \( t = 1.0 \) are shown in Figure 3.2(b). The process featured with \( \beta = 1.2, 1.4, 1.6, 1.8 \) is slightly more skewed to the right than that with \( \beta = 2.0 \). Furthermore, the solution continuously depends on the time and space fractional derivatives.
Table 3.1: Maximum errors at $t = 1$ with fixed time step $\tau = 0.01$

<table>
<thead>
<tr>
<th>$h$</th>
<th>LTM-MTM</th>
<th>FDM-MTM</th>
</tr>
</thead>
<tbody>
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<td>$\pi/8$</td>
<td>1.73E-02</td>
<td>1.98E-02</td>
</tr>
<tr>
<td>$\pi/16$</td>
<td>4.33E-03</td>
<td>7.05E-03</td>
</tr>
<tr>
<td>$\pi/32$</td>
<td>1.08E-03</td>
<td>4.00E-03</td>
</tr>
<tr>
<td>$\pi/64$</td>
<td>2.72E-04</td>
<td>3.28E-03</td>
</tr>
</tbody>
</table>

Table 3.2: Maximum errors at $t = 1$ with fixed space step $h = \pi/50$

<table>
<thead>
<tr>
<th>$\tau$</th>
<th>LTM-MTM</th>
<th>FDM-MTM</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1/10$</td>
<td>4.44E-04</td>
<td>3.43E-02</td>
</tr>
<tr>
<td>$1/25$</td>
<td>4.44E-04</td>
<td>1.31E-02</td>
</tr>
<tr>
<td>$1/50$</td>
<td>4.44E-04</td>
<td>6.60E-03</td>
</tr>
<tr>
<td>$1/100$</td>
<td>4.44E-04</td>
<td>3.44E-03</td>
</tr>
</tbody>
</table>

3.5 Conclusions

An analytical solution and two numerical schemes for approximating the TSS-FDE were derived under both homogeneous Dirichlet and Neumann boundary conditions. These solution techniques can be applied to other fractional partial differential equations. In future research, we will report the stability and convergence analyses of the proposed numerical methods.

Figure 3.2: Numerical solutions at $t = 1.0$ for the TSS-FDE (3.32)–(3.34) with $0 < \alpha < 1$, $\beta = 1.5$ (a); and $\alpha = 0.5$, $1 < \beta \leq 2$ (b).
Computationally efficient numerical methods for time and space fractional Fokker-Planck equations

4.1 Introduction

Brownian motion in the presence of an external force field $F(x) = -V'(x)$ is usually described in terms of the Fokker-Planck equation (FPE) [121]:

$$\frac{\partial W(x,t)}{\partial t} = \left[ \frac{\partial}{\partial x} \frac{V'(x)}{m\eta_1} + K_1 \frac{\partial^2}{\partial x^2} \right] W(x,t), \quad (4.1)$$

which defines the probability density function $W(x,t)$ to find the test particle at a certain position $x$ at a given time $t$; $m$ denotes the mass of the particle, $K_1$ is the diffusion constant associated with the transport process, and the friction coefficient $\eta_1$ is a measure for the interaction of the particle with its environment.

In many studies of diffusion processes where the diffusion takes place in a highly non-homogeneous medium, the traditional second-order FPE may not be adequate [13, 14]. The non-homogeneities of the medium may alter the laws of Markov diffusion in a fundamental way. In particular, the
corresponding probability density of the concentration field may have a heavier tail than the Gaussian density, and its correlation function may decay to zero at a much slower rate than the usual exponential rate of Markov diffusion, resulting in long-range dependence. This phenomenon is known as anomalous diffusion [16, 110].

The fractional Fokker-Planck equations have been recently treated by a number of authors and are found to be a useful approach for the description of transport dynamics in complex systems that are governed by anomalous diffusion and non-exponential relaxation patterns [110]. Fractional derivatives play a key role in modelling particle transport in anomalous diffusion. For the description of anomalous transport in the presence of an external field, Metzler and Klafter [110] introduced a time fractional extension of the FPE, namely the time-fractional Fokker-Planck equations (TFFPE). Benson et al. [13, 14] proposed a space-fractional Fokker-Planck equation (SFFPE) to simulate Lévy motion. Different assumptions on this probability density function lead to a variety of time- and space-fractional Fokker-Planck equations (TSFFPE) [110].

In this paper, we consider the following TSFFPE:

\[
\frac{\partial W(x,t)}{\partial t} = 0D_t^{1-\alpha}\left\{ \left[ \frac{\partial}{\partial x} V'(x) + K_\mu \frac{\partial}{\partial |x|} \right] W(x,t) + f(x,t) \right\},
\]

subject to the boundary and initial conditions

\[
W(a,t) = W(b,t) = 0, \quad 0 \leq t \leq T,
\]

\[
W(x,0) = W_0(x), \quad a \leq x \leq b,
\]

where \(K_\mu\) denotes the anomalous diffusion coefficient; \(m\) denotes the mass of the particle; \(\eta_\alpha\) is the generalised friction constant; and \(d(x) = V'(x)/m\eta_\alpha\) is known as the drift coefficient.

\(0D_t^{1-\alpha}\varphi\) denotes the Riemann-Liouville time fractional derivative (RLTFD) of order \(1 - \alpha\) \((0 < \alpha < 1)\) defined by [116]

\[
0D_t^{1-\alpha}\varphi = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{\varphi(x,\eta)}{(t-\eta)^{1-\alpha}} d\eta.
\]
The Riesz space fractional derivative (RSFD) of order $\mu \ (1 < \mu < 2)$ is defined by [48]

$$\frac{\partial^\mu W(x,t)}{\partial |x|^\mu} = -c_\mu (a D^\mu_x + x D^\mu_b) W(x,t), \quad (4.6)$$

where $c_\mu = 1/2 \cos(\pi \mu/2)$, $a D^\mu_x$ and $x D^\mu_b$ are the left and right Riemann-Liouville space fractional derivatives of order $\mu$ given by

$$a D^\mu_x W(x,t) = \frac{1}{\Gamma(2 - \mu)} \frac{\partial^2}{\partial x^2} \int_a^x W(\xi,t) d\xi \frac{(x - \xi)^{\mu-1}},$$

$$x D^\mu_b W(x,t) = \frac{1}{\Gamma(2 - \mu)} \frac{\partial^2}{\partial x^2} \int_x^b W(\xi,t) d\xi \frac{(\xi - x)^{\mu-1}}.$$

The FFPE has been investigated by a number of authors. So and Liu [140] studied the subdiffusive fractional Fokker-Planck equation of bistable systems. Metzler and Klafter [109] derived the explicit solution of the dispersive analogue of the Ornstein-Uhlenbeck process. Lenzi et al [73] derived a new exact class of solutions for the nonlinear fractional Fokker-Planck-like equation. Chen et al [24] proposed three different implicit approximations for the TFFPE and proved these approximations are unconditionally stable and convergent. Benson et al [13, 14] derived the analytic solutions of the SFFPE in some special cases. Liu et al [78] considered a SFFPE with instantaneous source, and transformed the SFFPE into a system of ordinary differential equations (method of lines) that was then solved using backward differentiation formulas. Zhuang et al [169] presented an implicit numerical method for the TSFFPE and discussed its stability and convergence.

Recently, Marseguerra and Zoia [102] and Fulger et al [42] presented an alternative numerical solution strategy based on Monte Carlo simulations. In this method, they simulated the fractional kinetics equations via continuous-time random walks with different assumptions on the distributions of jumps in space and distributions of waiting times. However, one notes from Fulger et al [42] that this strategy is rather computationally expensive requiring CPU time 437 seconds (for $10^7$ runs with waiting time 0.01 and number of jumps 74 per run for $t \in [0, 2]$) to compute the solution of the time-space fractional diffusion equation.

Therefore, numerical methods for TSFFPE are quite limited, and published papers on the numerical solution of the TSFFPE are sparse. This motivates us to consider effective numerical
methods for the TSFFPE. One of the highlights of our proposed numerical methods is its computational efficiency. The stability and convergence analyses of these methods will be reported in future work by the authors.

The remainder of this paper is structured as follows. In Section 4.2, three numerical methods are proposed to deal with the Riesz space fractional derivative (RSFD): the $L^2$-approximation method, the shifted Grünwald method, and the matrix transform method (MTM). In Section 4.3, the Riemann-Liouville time fractional derivative (RLTFD) is approximated by the Grünwald method. In Section 4.4, the TSFFPE is transformed into a system of ordinary differential equations (ODE), which is then solved by a fractional implicit trapezoidal method (FITM). Finally, some numerical examples are given in Section 4.5.

4.2 Numerical approximation methods of the RSFD

Assume that the spatial domain is $[a, b]$. The mesh is $M$ equal intervals $\{[x_{l-1}, x_l]\}_{l=1}^M$ of $h = (b - a)/M$ and $x_l = a + lh$ for $0 \leq l \leq M$. Let $W_l$ denote the numerical approximation of $W(x_l, t)$.

4.2.1 $L^2$-approximation method for the RSFD

Using the link between the Riemann-Liouville and Grünwald-Letnikov definitions, the following $L^2$-approximation of the RSFD can be obtained [78]:

$$
\frac{\partial^\mu W_l}{\partial |x|^\mu} \approx -\frac{h^{-\mu}}{2 \cos\left(\frac{\pi \mu}{2}\right) \Gamma(3-\mu)} \left\{ \frac{(1-\mu)(2-\mu)}{\mu} W_0 
+ \frac{(2-\mu)}{(M-1)\mu} W_M + \frac{(2-\mu)}{(M-l)\mu} (W_M - W_{M-1}) 
+ \sum_{i=0}^{M-l-1} b_i(W_{l+i+1} - 2W_{l+i} + W_{l+i+1}) \right\},
$$

(4.7)

where $b_i = (i + 1)^{2-\mu} - i^{2-\mu}$, $i = 0, \ldots, M$. 

4.2 Numerical approximation methods of the RSFD

4.2.2 Shifted Grünwald approximation method for the RSFD

The shifted Grünwald formula for discretising the two-sided fractional derivative was proposed by Meerschaert and Tadjeran [107], and it was shown that the standard (i.e., unshifted) Grünwald formula to discretise the fractional diffusion equation results in an unstable finite difference scheme regardless of whether the resulting finite difference method is an explicit or an implicit scheme. Hence, in this section, we discretise the RSFD using the following shifted Grünwald approximation:

$$\frac{\partial^\mu W_i}{\partial |x|^\mu} \approx -\frac{h^{-\mu}}{2 \cos\left(\frac{\pi \mu}{2}\right)} \left[ \sum_{i=0}^{l+1} w_{\mu}^i W_{i-l+1} + \sum_{i=0}^{M-l+1} w_{\mu}^i W_{i+l-1} \right]$$

where the coefficients are defined by

$$w_{\mu}^0 = 1, \quad w_{\mu}^i = (-1)^i \frac{\mu(\mu-1)...(\mu-i+1)}{i!}, \quad i = 1, 2, ..., M.$$

4.2.3 Matrix transform method for the RSFD

We note that the Riesz fractional derivative is equivalent to the fractional power of the Laplace operator under homogeneous Dirichlet boundary conditions [150]. Hence, the RSFD can be approximated and written in the following matrix form [60]:

$$\frac{\partial^\mu \bar{W}}{\partial |x|^\mu} = -(-\Delta)^{\frac{\mu}{2}} \bar{W} \approx -\frac{1}{h^\mu} A^\frac{\mu}{2} \bar{W},$$

where $\bar{W} \in \mathbb{R}^{(M-1) \times 1}$ and $A \in \mathbb{R}^{(M-1) \times (M-1)}$ are given respectively by

$$\bar{W} = \begin{bmatrix} W_1 \\ \vdots \\ W_{M-1} \end{bmatrix}, \quad A = \begin{bmatrix} 2 & -1 \\ -1 & 2 & -1 \\ & \ddots & \ddots & \ddots \\ & & -1 & 2 \end{bmatrix}.$$
The matrix $A$ is symmetric positive definite (SPD), and therefore there exits a nonsingular matrix $P \in \mathbb{R}^{(M-1) \times (M-1)}$ such that

$$A = P \Lambda P^T,$$

where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_{M-1})$, $\lambda_i (i = 1, 2, \ldots, M - 1)$ being the eigenvalues of $A$.

Thus, we obtain

$$\frac{\partial^\mu \bar{W}}{\partial |x|^\mu} \approx -\frac{1}{h^\mu} P \Lambda^\mu P^T \bar{W}.$$  

(4.10)

### 4.3 Numerical approximation method of the RLTFD

Suppose that the function $W(x, t)$ is $n - 1$ times continuously differentiable in the interval $[0, T]$ and that $W^{(n)}(x, t)$ is integrable in $[0, T]$. Then for every $\alpha$ ($0 \leq n - 1 < \alpha \leq n, n \in \mathbb{N}$), the Riemann-Liouville fractional derivative exists and coincides with the Grünwald-Letnikov derivative. This allows the use of the Riemann-Liouville definition during problem formulation, and then the Grünwald-Letnikov definition for obtaining a numerical solution [78]. The fractional Grünwald-Letnikov derivative definition with order $1 - \alpha$ is given by [116]

$$0D_t^{1-\alpha} W(x, t) = \lim_{\tau \to 0} \tau^{\alpha-1} \sum_{j=0}^{k} (-1)^j \binom{1-\alpha}{j} W(x, t_k - j\tau)$$

$$= \tau^{\alpha-1} \sum_{j=0}^{k} w_j^{1-\alpha} W(x, t_k - j\tau) + O(\tau^p),$$

(4.11)

where $\tau = \frac{T}{N}$, $t_j = j\tau$, $w_0^{1-\alpha} = 1$, $w_j^{1-\alpha} = (-1)^j \frac{(1-\alpha)(-\alpha)\ldots(2-\alpha-j)}{j!}$, for $j = 1, 2, \ldots, N$.

This formula is not unique because there are many different valid choices for $w_j^{1-\alpha}$ that lead to approximations of different order $p$ [74, 96]. The definition (4.11) provides order $p = 1$.

### 4.4 Fractional Implicit Trapezoidal Method for the TSFFPE

The $L2$-approximation method, the shifted Grünwald method, and the matrix transform method (MTM) are used to approximate the RSFD, the Grünwald method is used to approximate the
4.4 Fractional Implicit Trapezoidal Method for the TSFFPE

RLTFD, and the backward difference scheme if \( d(x) < 0 \) (the forward difference scheme if \( d(x) > 0 \)) is used to approximate the first order spatial derivative, the TSFFPE can be cast into the following ordinary differential equation (ODE):

\[
\frac{dW(x_l, t)}{dt} = 0D_t^{1-\alpha}\varphi(W(x_l, t)).
\] (4.12)

In this section, a fractional implicit trapezoidal method (FITM) is used to integrate (4.12). Let \( W_{l}^{k} \) denote the numerical approximation of \( W(x_l, t_{k}) \). The FITM can be written in the following form:

\[
W_{l}^{k+1} = W_{l}^{k} + \frac{\tau}{2} \left\{ \sum_{j=0}^{k} w_{j}^{1-\alpha}\varphi(W_{l}^{k-j}) + \sum_{j=1}^{k+1} w_{j}^{1-\alpha}\varphi(W_{l}^{k-j+1}) + \varphi(W_{l}^{k+1}) \right\}.
\] (4.13)

Hence, we can rewrite (4.13) in the matrix form:

\[
T \bar{W}_{k+1}^{l} = \bar{R},
\] (4.14)

where \( T \in \mathbb{R}^{(M-1) \times (M-1)} \), \( \bar{R} \in \mathbb{R}^{(M-1) \times 1} \), and \( \bar{W}_{k+1}^{l} \in \mathbb{R}^{(M-1) \times 1} \) for \( k = 0, \ldots, N - 1 \).

4.4.1 FITM with L2-approximation

When the FITM with \( L2 \)-approximation is used to solve the TSFFPE, the term \( \varphi(W_{l}^{k-j}) \) can be written in the following form:

\[
\varphi(W_{l}^{k-j}) = \frac{d_{l}W_{l}^{k-j} - d_{l-1}W_{l-1}^{k-j}}{h} - \frac{R_{n}^{\mu}h^{-\mu}}{2\cos(\frac{\mu\pi}{2})\Gamma(3-\mu)}
\]

\[
\left\{ \left( \frac{1-\mu}{\mu} \right) (2-\mu) W_{0}^{k-j} + \frac{(2-\mu)}{\mu-1} (W_{1}^{k-j} - W_{0}^{k-j}) \right. \\
+ \sum_{i=0}^{l-1} b_{i}(W_{l-i+1}^{k-j} - 2W_{l-i}^{k-j} + W_{l-i-1}^{k-j}) \\
+ \frac{(1-\mu)(2-\mu)}{(M-l)^{\mu}} W_{M}^{k-j} + \frac{(2-\mu)}{(M-l)^{\mu-1}} (W_{M}^{k-j} - W_{M-1}^{k-j}) \\
+ \sum_{i=0}^{M-l-1} b_{i}(W_{l+i-1}^{k-j} - 2W_{l+i}^{k-j} + W_{l+i+1}^{k-j}) \right\} + f_{l}^{k-j},
\] (4.15)
and the term $\varphi(W_t^{k+1})$ can be expressed as

$$\varphi(W_t^{k+1}) = \frac{d_l W_t^{k+1} - d_{l-1} W_t^{k+1}}{h} - \frac{K_0^\mu h^{-\mu}}{2 \cos\left(\frac{\pi \mu}{2}\right) \Gamma(3 - \mu)} \left\{ \frac{(1 - \mu)(2 - \mu)}{\mu} W_0^{k+1} + \frac{(2 - \mu)}{\mu - 1} (W_1^{k+1} - W_0^{k+1}) + \sum_{i=0}^{l-1} b_i (W_{l-i+1}^{k+1} - 2W_{l-i}^{k+1} + W_{l-i-1}^{k+1}) \\
+ \frac{(1 - \mu)(2 - \mu)}{(M - l)^\mu} W_M^{k+1} + \frac{(2 - \mu)}{(M - l)^{\mu-1}} (W_M^{k+1} - W_{M-1}^{k+1}) + \sum_{i=0}^{M-l-1} b_i (W_{M-i}^{k+1} - 2W_{M-i+1}^{k+1} + W_{M-i+2}^{k+1}) \right\} + f_l^{k+1}$$

(4.16)

Hence, the coefficient matrix $T$ and vector $\tilde{R}$ can be obtained from the left side and the right side of the following equation respectively:

$$W_t^{k+1} - \frac{x_\alpha}{2} \psi(W_t^{k+1}) = W_t^k + \frac{x_\alpha}{2} \left\{ \sum_{j=0}^{k} w_1^{1-\alpha} \varphi(W_t^{k-j}) + \sum_{j=1}^{k+1} w_1^{1-\alpha} \varphi(W_t^{k-j+1}) + f_l^{k+1} \right\},$$

(4.17)

for $l = 1, \ldots, M - 1$.

### 4.4.2 FITM with Shifted Grünwald method

When the FITM with Shifted Grünwald method is used to solve the TSFFPE, the term $\varphi(W_t^{k-j})$ can be written in the following form:

$$\varphi(W_t^{k-j}) = \frac{d_l W_t^{k-j} - d_{l-1} W_t^{k-j}}{h} - \frac{K_0^\mu h^{-\mu}}{2 \cos\left(\frac{\pi \mu}{2}\right)} \left[ \sum_{i=0}^{l+1} w_1^\mu W_t^{k-j} + \sum_{i=0}^{M-l+1} w_1^\mu W_t^{k-j} \right] + f_l^{k-j},$$

(4.18)
and the term $\varphi(W_{l}^{k+1})$ can be expressed as:

$$
\varphi(W_{l}^{k+1}) = \frac{d_{l}W_{l}^{k+1} - d_{l-1}W_{l-1}^{k+1}}{h} - \frac{K_{1}^{\mu}h^{-\mu}}{2\cos(\frac{\pi\mu}{2})}
$$

$$
\left[ \sum_{i=0}^{l+1} w_{i}^{\mu}W_{l-i+1}^{k+1} + \sum_{i=0}^{M-l+1} w_{i}^{\mu}W_{l+i-1}^{k+1} \right] + f_{l}^{k+1}, \quad (4.19)
$$

where $w_{0}^{\mu} = 1$, $w_{i}^{\mu} = (-1)^{i} \frac{\mu(\mu-1)\ldots(\mu-i+1)}{i!}$, for $i = 1, 2, ..., M$.

Hence, the coefficient matrix $T = (t_{li})_{(M-1)\times(M-1)}$ and vector $\bar{R} = (r_{l})_{(M-1)}$ are defined by

$$
t_{li} = \begin{cases} 
R_{\alpha}^{\mu}w_{l-i+1}, & 1 \leq i < l - 1, \\
R_{\alpha}^{\mu}(w_{0} + w_{2}) + \tau_{\alpha}^{\mu}d_{l-i+1}, & i = l - 1, \\
1 + 2R_{\alpha}^{\mu}w_{1} - \tau_{\alpha}^{\mu}d_{l}, & i = l \\
R_{\alpha}^{\mu}(w_{0} + w_{2}), & i = l + 1, \\
R_{\alpha}^{\mu}w_{l-i+1}, & l + 1 < i \leq M - 1, 
\end{cases} \quad (4.20)
$$

$$
r_{l} = W_{l}^{k} + \frac{\tau_{\alpha}^{\mu}}{2} \left\{ \sum_{j=0}^{k} w_{j}^{1-\alpha}\varphi(W_{l}^{k-j}) + \sum_{j=1}^{k+1} w_{j}^{1-\alpha}\varphi(W_{l}^{k-j+1}) + f_{l}^{k+1} \right\}, \quad (4.21)
$$

where $R_{\alpha}^{\mu} = \frac{K_{1}^{\mu}\tau_{\alpha}^{\mu}h^{-\mu}}{4\cos(\frac{\pi\mu}{2})}$.

### 4.4.3 FITM with matrix transform method

The FITM with matrix transform method for solving the TSFFPE can be written in the following form:

$$
\hat{W}_{l}^{k+1} = \hat{W}_{l}^{k} + \frac{\tau_{\alpha}^{\mu}}{2} \left\{ \sum_{j=0}^{k} w_{j}^{1-\alpha}(\Phi \hat{W}_{l}^{k-j} + \hat{F}_{l}^{k-j}) \\
+ \sum_{j=1}^{k+1} w_{j}^{1-\alpha}(\Phi \hat{W}_{l}^{k+1-j} + \hat{F}_{l}^{k+1-j}) + \Phi \hat{W}_{l}^{k+1} + \hat{F}_{l}^{k+1} \right\}, \quad (4.22)
$$
The matrix \( \Phi \in \mathbb{R}^{(M-1)\times(M-1)} \) can be written as

\[
\Phi = -\eta \mu (P \Lambda^{\mu/2} P^T) + \frac{1}{h} D,
\]

(4.23)

where \( \eta = \frac{K}{n} \), \( D \in \mathbb{R}^{(M-1)\times(M-1)} \), \( F_{k-j} \in \mathbb{R}^{(M-1)\times1} \).

\[
D = \begin{bmatrix}
    d_1 & & & & \\
    -d_1 & d_2 & & & \\
    & -d_2 & d_3 & & \\
    & & \ddots & \ddots & \\
    & & & -d_{M-2} & d_{M-1}
\end{bmatrix},
\]

\[
F_{k-j} = \begin{bmatrix}
    f_{1-k-j} \\
    \vdots \\
    f_{M-k-j}
\end{bmatrix}.
\]

Hence, the coefficient matrix \( T \) and vector \( \bar{R} \) are defined by

\[
T = I - \frac{\tau}{2} \Phi,
\]

(4.24)

\[
\bar{R} = \bar{W}^k + \frac{\tau}{2} \left\{ \sum_{j=0}^{k} w^{1-\alpha}_{j} (\Phi \bar{W}^{k-j} + F^{k-j}) + \sum_{j=1}^{k+1} w^{1-\alpha}_{j} (\Phi \bar{W}^{k+1-j} + F^{k+1-j}) + F^{k+1} \right\}. 
\]

(4.25)

### 4.5 Numerical examples

To demonstrate the effectiveness of these numerical methods for the solving time-space fractional Fokker-Planck equation, we consider the following two examples.

**Example 4.1.** Consider the following TSFFPE:

\[
\frac{\partial W(x,t)}{\partial t} = \alpha D^{1-\alpha} \left\{ -\nu \frac{\partial}{\partial x} + K^{\mu} \frac{\partial^{\mu}}{\partial |x|^{\mu}} \right\} W(x,t) + f(x,t),
\]

(4.26)

\[
W(a,t) = W(b,t) = 0, \quad 0 \leq t \leq T,
\]

(4.27)

\[
W(x,0) = K^{\mu}(x-a)^2(b-x)^2, \quad a \leq x \leq b,
\]

(4.28)
where

\[
4.5 \text{ Numerical examples} \quad f(x,t) = (1 + \alpha) v \Gamma(1 + \alpha) t (x - a)^2 (b - x)^2
\]
\[
+ \frac{K_\alpha}{2} \frac{K_\alpha + vt^{1+\alpha}}{2 \cos(\frac{\pi \mu}{2})} [g(x - a) + g(b - x)]
\]
\[
+ 2v(K_\alpha + vt^{1+\alpha})(x - a)(b - x)(a + b - 2x),
\]
\[
g(x) = \frac{4!}{\Gamma(5 - \mu)} x^{4-\mu} - 2(b - a) \frac{3!}{\Gamma(4 - \mu)} x^{3-\mu}
\]
\[
+ (b - a)^2 \frac{2}{\Gamma(3 - \mu)} x^{2-\mu}.
\]

The exact solution is

\[
W(x,t) = (K_\alpha + vt^{1+\alpha})(x - a)^2 (b - x)^2,
\]

which can be verified by direct fractional differentiation of the given solution, and substituting into the fractional differential equation. The initial condition is clearly satisfied. In this example, we take \( a = 0, b = 1, K_\alpha = 25, v = 1, \tau = 0.01, h = 1/64 \). Figures 4.1–4.3 show the comparison of the exact and numerical solutions of the FITM with the \( L^2 \)-approximation method, the shifted Gr"unwald method, and the matrix transform method (MTM) when \( \alpha = 0.8, \mu = 1.9 \) and \( \alpha = 0.6, \mu = 1.8 \) at \( t = 1 \); and when \( \alpha = 0.9, \mu = 1.9 \) at \( t = 1, 3, 5 \), respectively. It can be seen that the numerical solutions are in excellent agreement with the exact solution.

It is also worthwhile mentioning that, in comparison to the Monte Carlo simulations reported in [42], our numerical simulations are computationally efficient, requiring only a few seconds to complete execution and output the results (see Table 4.1).

**Example 4.2.** Consider the following TSFFPE:

\[
\frac{\partial W(x,t)}{\partial t} = aD_t^{1-\alpha} \left[ -v \frac{\partial}{\partial x} + K_\alpha \frac{\partial^\mu}{\partial |x|^\mu} \right] W(x,t),
\]

\[
W(a,t) = W(b,t) = 0, \quad 0 \leq t \leq T,
\]

\[
W(x,0) = c_0 \delta(x), \quad a \leq x \leq b,
\]

In this example, we take \( a = -10, b = 10, K_\alpha = 1, v = 1, \tau = 0.01, h = 0.2 \). The evolution results of the FITM with shifted Gr"unwald method when \( \alpha = 1.0, \mu = 2.0; \alpha = 0.9, \mu = 1.9; \)
Figure 4.1: Comparison of numerical and analytic solutions at \( t = 1 \) for the TSFFPE (4.26)-(4.28) with \( \alpha = 0.8, \mu = 1.9 \).

Table 4.1: Total CPU time \( T \) in seconds of the three numerical schemes given in Section 4 to approximate the solution of the TSFFPE (4.26)-(4.28) at \( t = 1 \) with \( \alpha = 0.6, \mu = 1.8 \).

<table>
<thead>
<tr>
<th>( \tau )</th>
<th>( h )</th>
<th>T(L2)</th>
<th>T(Shifted Grünwald)</th>
<th>T(MTM)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/20</td>
<td>1/16</td>
<td>0.08</td>
<td>0.08</td>
<td>0.06</td>
</tr>
<tr>
<td>1/50</td>
<td>1/32</td>
<td>0.86</td>
<td>0.78</td>
<td>0.77</td>
</tr>
<tr>
<td>1/100</td>
<td>1/64</td>
<td>7.03</td>
<td>6.31</td>
<td>6.30</td>
</tr>
</tbody>
</table>

\( \alpha = 0.8, \mu = 1.8; \alpha = 0.6, \mu = 1.8 \) and \( \alpha = 0.4, \mu = 1.5 \) at \( t = 1.25, 2.5, 3.75, 5.0 \) are listed in Figures 4.4-4.8, respectively. Figures 4.4-4.8 show that the system exhibits anomalous diffusion behaviours. The noteworthy features are the appearance of cusps and a heavy tail of the probability density function \( W \) that decays when \( 0 < \alpha < 1 \) and \( 1 < \mu < 2 \).
4.5 Numerical examples

Figure 4.2: Comparison of numerical and analytic solutions at $t = 1$ for the TSFFPE (4.26)-(4.28) with $\alpha = 0.6$, $\mu = 1.8$.

Figure 4.3: Comparison of numerical and analytic solutions at $t = 1, 3, 5$ for the TSFFPE (4.26)-(4.28) with $\alpha = 0.9$, $\mu = 1.9$. 
Figure 4.4: The numerical solutions of $W(x,t)$ for the TSFFPE \((4.30)-(4.32)\) with $\alpha = 1.0$, $\mu = 2.0$ at $t = 1.25, 2.5, 3.75, 5.0$.

Figure 4.5: The numerical solutions of $W(x,t)$ for the TSFFPE \((4.30)-(4.32)\) with $\alpha = 0.9$, $\mu = 1.9$ at $t = 1.25, 2.5, 3.75, 5.0$. 
Figure 4.6: The numerical solutions of $W(x, t)$ for the TSFFPE (4.30)-(4.32) with $\alpha = 0.8$, $\mu = 1.8$ at $t = 1.25, 2.5, 3.75, 5.0$.

Figure 4.7: The numerical solutions of $W(x, t)$ for the TSFFPE (4.30)-(4.32) with $\alpha = 0.6$, $\mu = 1.8$ at $t = 1.25, 2.5, 3.75, 5.0$. 
Figure 4.8: The numerical solutions of $W(x,t)$ for the TSFFPE (4.30)-(4.32) with $\alpha = 0.4$, $\mu = 1.5$ at $t = 1.25, 2.5, 3.75, 5.0$. 
Stability and convergence of an effective numerical method for the time-space fractional Fokker-Planck equation with a nonlinear source term

5.1 Introduction

The Fokker-Planck equation (FPE) has commonly been used to describe the Brownian motion of particles. Normal diffusion in an external force field is often modelled in terms of the following Fokker-Planck equation (FPE) \[ \frac{\partial u(x,t)}{\partial t} = \left[ \frac{\partial}{\partial x} V'(x) m \eta_1 + K_1 \frac{\partial^2}{\partial x^2} \right] u(x,t), \] (5.1)

where \( m \) is the mass of the diffusing test particle, \( \eta_1 \) denotes the fraction constant characterising the interaction between the test particle and its embedding, and the force is related to the external potential through \( F(x) = \frac{dV(x)}{dx} \). The FPE (5.1) is well-studied for a variety of potential types, and the respective results have found wide application. In many studies of diffusion processes where the diffusion takes place in a highly non-homogeneous medium, the
traditional FPE may not be adequate [13, 14]. The non-homogeneities of the medium may alter the laws of Markov diffusion in a fundamental way. In particular, the corresponding probability density of the concentration field may have a heavier tail than the Gaussian density, and its correlation function may decay to zero at a much slower rate than the usual exponential rate of Markov diffusion, resulting in long-range dependence. This phenomenon is known as anomalous diffusion [16]. Fractional derivatives play a key role in modelling particle transport in anomalous diffusion including the space fractional Fokker-Planck (advection-dispersion) equation describing Lévy flights, the time fractional Fokker-Planck equation depicting traps, and the time-space fractional equation characterising the competition between Lévy flights and traps [109, 160]. Different assumptions on this probability density function lead to a variety of time-space fractional Fokker-Planck equations (TSFFPE).

TSFFPE has been successfully used for modelling relevant physical processes. When the fractional differential equation is used to describe the asymptotic behaviour of continuous time random walks, its solution corresponds to the Lévy walks, generalising the Brownian motion to the Lévy motion. The following space fractional Fokker-Planck equation has been considered [13, 14, 78]

\[
\frac{\partial u(x,t)}{\partial t} = -v \frac{\partial u(x,t)}{\partial x} + K_\mu \left[ c_+ aD^\mu_x u(x,t) + c_- xD^\mu_b u(x,t) \right],
\]

(5.2)

where \( v \) is the drift of the process, that is, the mean advective velocity; \( K_\mu \) is the coefficient of dispersion; \( aD^\mu_x \) and \( xD^\mu_b \) are the left and right Riemann-Liouville space fractional derivatives of order \( \mu \) given by

\[
aD^\mu_x u(x,t) = \frac{1}{\Gamma(2-\mu)} \frac{\partial^2}{\partial x^2} \int_a^x \frac{u(\xi,t)d\xi}{(x-\xi)^{\mu-1}},
\]

\[
xD^\mu_b u(x,t) = \frac{1}{\Gamma(2-\mu)} \frac{\partial^2}{\partial x^2} \int_x^b \frac{u(\xi,t)d\xi}{(\xi-x)^{\mu-1}},
\]

c_+ \text{ and } c_- \text{ indicate the relative weight of transition probability; Benson et al. [13, 14] took } c_+ = \frac{1}{2} + \frac{\beta}{2} \text{ and } c_- = \frac{1}{2} - \frac{\beta}{2}, \text{ } (-1 \leq \beta \leq 1), \text{ which indicate the relative weight forward versus backward transition probability. If } c_+ = c_- = -c_\mu = -\frac{1}{2 \cos(\pi \mu/2)}, \text{ Eq. (5.2) can be rewritten}
in the following form:

\[
\frac{\partial u(x,t)}{\partial t} = -v \frac{\partial u(x,t)}{\partial x} + K \mu \frac{\partial^\mu u(x,t)}{\partial |x|^\mu},
\]

where \( \frac{\partial^\mu}{\partial |x|^\mu} \) is the symmetric space fractional derivative of order \( \mu \) (1 < \( \mu \) ≤ 2). This is also referred to as the Riesz derivative \([48]\), which contains a left Riemann-Liouville derivative \( (_a D_x^\mu) \) and a right Riemann-Liouville derivative \( (_b D_y^\mu) \), namely

\[
\frac{\partial^\mu}{\partial |x|^\mu} u(x,t) = -c_\mu (_a D_x^\mu + _x D_y^\mu) u(x,t).
\]

As a model for subdiffusion in the presence of an external field, a time fractional extension of the FPE has been introduced as the time fractional Fokker-Planck equation (TFFPE) \([25, 109]\)

\[
\frac{\partial u(x,t)}{\partial t} = 0_{D_t^{1-\alpha}} \left[ \frac{\partial}{\partial x} V'(x) + K_{\alpha} \frac{\partial^2}{\partial x^2} \right] u(x,t),
\]

where the Riemann-Liouville operator \( 0_{D_t^{1-\alpha}} \), (0 < \( \alpha \) < 1) is defined through its operation

\[
0_{D_t^{1-\alpha}} u(x,t) = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{u(x,\eta)}{(t-\eta)^{1-\alpha}} d\eta.
\]

Yuste and Acedo \([158]\) proposed an explicit finite difference method and a new von Neumann-type stability analysis for the anomalous subdiffusion equation (5.5) with \( V'(x) = 0 \). However, they did not give a convergence analysis and pointed out the difficulty of this task when implicit methods are considered. Langlands and Henry \([71]\) also investigated this problem and proposed an implicit numerical L1-approximation scheme, and discussed the accuracy and stability of this scheme. However, the global accuracy of the implicit numerical scheme has not been derived and it seems that the unconditional stability for all \( \alpha \) in the range 0 < \( \alpha \) ≤ 1 has not been established. Recently, Chen and Liu et al. \([22]\) presented a Fourier method for the anomalous sub-diffusion equation, and they gave the stability analysis and the global accuracy analysis of the difference approximation scheme. Zhuang and Liu et al. \([166]\) also proposed an implicit numerical method and an analytical technique for the anomalous sub-diffusion equation. Chen and Liu et al. \([20]\) proposed implicit and explicit numerical approximation schemes
for the Stokes’ first problem for a heated generalised second grade fluid with fractional derivatives. The stability and convergence of the numerical scheme are discussed using a Fourier method. A Richardson extrapolation technique for improving the order of convergence of the implicit scheme is presented. However, effective numerical methods and error analysis for the time-space fractional Fokker-Planck equation with a nonlinear source term are still in their infancy and are open problems.

Equation (5.5) can be written as the following equivalent form [24]:

\[
0D_t^\alpha u(x, t) - \frac{u(x, 0)t^{-\alpha}}{\Gamma(1 - \alpha)} = \left[ \frac{\partial}{\partial x} V'(x) + K_\alpha \frac{\partial^2}{\partial x^2} \right] u(x, t). \tag{5.6}
\]

By noting that [24]:

\[
\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = 0D_t^\alpha u(x, t) - \frac{u(x, 0)t^{-\alpha}}{\Gamma(1 - \alpha)}, \tag{5.7}
\]

we arrive at

\[
\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \left[ \frac{\partial}{\partial x} V'(x) + K_\alpha \frac{\partial^2}{\partial x^2} \right] u(x, t), \tag{5.8}
\]

where \(\frac{\partial^\alpha u(x, t)}{\partial t^\alpha}\) is the Caputo time fractional derivative (CTFD) of order \(\alpha\) \((0 < \alpha < 1)\) with starting point at \(t = 0\) defined by [116]:

\[
\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{1}{\Gamma(1 - \alpha)} \int_0^t \frac{\partial u(x, \eta)}{\partial \eta} \frac{d\eta}{(t - \eta)^\alpha}. \tag{5.9}
\]

The time-space fractional Fokker-Planck equation (TSFFPE), which describes the competition between subdiffusion and Lévy flights, is given by [109]:

\[
\frac{\partial u(x, t)}{\partial t} = 0D_t^{1-\alpha} \left[ \frac{\partial}{\partial x} V'(x) + K_\mu \frac{\partial^\mu}{\partial |x|^\mu} \right] u(x, t), \tag{5.10}
\]

or

\[
\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \left[ \frac{\partial}{\partial x} V'(x) + K_\mu \frac{\partial^\mu}{\partial |x|^\mu} \right] u(x, t), \tag{5.11}
\]

where \(K_\mu\) denotes the anomalous diffusion coefficient.
Schot et al. [134] investigated a fractional diffusion equation that employs time and space fractional derivatives by taking an absorbent (or source) term and an external force into account, which can be described by the following time-space fractional Fokker-Plank equation with an absorbent term and a linear external force:

$$\frac{\partial^{\alpha} u(x,t)}{\partial t^{\alpha}} = - \frac{\partial}{\partial x} \left[ F(x) u(x,t) \right] + K_\alpha^\mu \frac{\partial^\mu}{\partial |x|^\mu} u(x,t) - \int_0^t r(t-\eta) u(x,\eta) d\eta,$$  \hspace{1cm} (5.12)

where $F(x)$ is the external force and $r(t)$ is a time-dependent absorbent term, which may be related to a reaction diffusion process.

The fractional Fokker-Planck equations (FFPE) have been recently treated by many authors and are presented as a useful approach for the description of transport dynamics in complex systems that are governed by anomalous diffusion and non-exponential relaxation patterns. The analytical solution of FFPE is only possible in simple and special cases [13, 14, 73] and the analytical solution provides a general representation in terms of the Green functions. We note that the representation of the Green functions is mostly expressed as convergent expansions in negative and positive power series. These special functions are not suitable for numerical evaluation when $x$ is sufficiently small or sufficiently large. Therefore, a new numerical strategy is important for solving these equations. Although numerical methods for the time fractional Fokker-Planck type equation, the space fractional Fokker-Plank type equation, and the time-space fractional Fokker-Planck type equation have been considered [24, 78, 169], numerical methods and stability and convergence analysis for the FFPE are quite limited and difficult. In fact, published papers on the numerical methods for the FFPE are sparse. We are unaware of any other published work on numerical methods for the time-space fractional Fokker-Planck type equation with a nonlinear source term. This motivates us to consider an effective numerical method for the time-space fractional Fokker-Planck equation with a nonlinear source term and to investigate its stability and convergence.

In this paper, we consider the following time-space fractional Fokker-Planck equation with a nonlinear source term (TSFFPE-NST):

$$\frac{\partial^{\alpha} u(x,t)}{\partial t^{\alpha}} = \left[ \frac{\partial}{\partial x} \frac{V'(x)}{m\eta_0} + K_\alpha^\mu \frac{\partial^\mu}{\partial |x|^\mu} \right] u(x,t) + s(u, x, t),$$  \hspace{1cm} (5.13)
subject to the boundary and initial conditions

\begin{align}
  u(a, t) &= u(b, t) = 0, \quad 0 \leq t \leq T, \\
  u(x, 0) &= u_0(x), \quad a \leq x \leq b,
\end{align}

(5.14), (5.15)

where \( p(x) = \frac{V'(x)}{m \eta} \) is known as the drift coefficient. The nonlinear source (or absorbent) term \( s(u, x, t) \) is assumed to satisfy the Lipschitz condition

\[ \| s(u, x, t) - s(v, x, t) \| \leq L \| u - v \| . \]

(5.16)

Let \( X \) be a Banach space with associated norm \( \| u \| \). We say that \( s : X \to X \) is globally Lipschitz continuous if for some \( L > 0 \), we have \( \| s(u) - s(v) \| \leq L \| u - v \| \) for all \( u, v \in X \), and is locally Lipschitz continuous, if the latter holds for \( \| u \|, \| v \| \leq M \) with \( L = L(M) \) for any \( M > 0 \) [9].

Let \( \Omega = [a, b] \times [0, T] \). In this paper, we suppose that the continuous problem (5.13)-(5.15) has a smooth solution \( u(x, t) \in C^{1+\mu, 2}_{x,t}(\Omega) \).

The rest of this paper is organised as follows. In Section 5.2, the Caputo time fractional derivative (CTFD) and the Riesz space fractional derivative (RSFD) are approximated by the L1-algorithm and the shifted Grünwald method, respectively. An effective numerical method (ENM) for solving the TSFFPE-NST (5.13)-(5.15) is proposed. The stability and convergence of the ENM are discussed in Sections 5.3 and 5.4, respectively. In Section 5.5, numerical experiments are carried out to support the theoretical analysis. Finally, some conclusions are drawn in Section 5.6.

### 5.2 An effective numerical method for the TSFFPE-NST

In this section, we present an effective numerical method to simulate the solution behaviour of the TSFFPE-NST (5.13)-(5.15). Let \( x_l = lh \ (l = 0, 1, \ldots, M) \) and \( t_n = n\tau \ (n = 0, 1, \ldots, N) \), where \( h = (b - a)/M \) and \( \tau = T/N \) are the spatial and temporal steps, respectively.
5.2 An effective numerical method for the TSFFPE-NST

Firstly, adopting the L1-algorithm [114], we discretise the Caputo time fractional derivative as

$$\frac{\partial^\alpha u(x, t_{n+1})}{\partial t^\alpha} = \frac{\tau^{-\alpha}}{\Gamma(2 - \alpha)} \sum_{j=0}^{n} b_j [u(x, t_{n+1-j}) - u(x, t_n-j)] + O(\tau^{1+\alpha}), \quad (5.17)$$

where $b_j = (j + 1)^{1-\alpha} + j^{1-\alpha}$, $j = 0, 1, 2, \ldots, N - 1$.

For the symmetric Riesz space fractional derivative, we use the following shifted Grünwald approximation [107]:

$$\frac{\partial^\mu u(x_1, t)}{\partial |x|^\mu} = \frac{-h^{-\mu}}{2 \cos(\frac{\pi \mu}{2})} \left[ \sum_{i=0}^{l+1} w_i u(x_{i-1}, t) + \sum_{i=0}^{M-l+1} w_i u(x_{i+1}, t) \right] + O(h^q) \quad (5.18)$$

where the coefficients are defined by

$$w_0 = 1, \quad w_i = (-1)^i \frac{i!}{\mu(i-1)!} \frac{\mu(i) \cdots (\mu + i)}{i!}, \quad i = 1, 2, \ldots, M.$$  

This formula is not unique because there are many different valid choices for $w_i$ that lead to approximations of different order $q$ [74]. The definition (5.18) provides order $q = 1$.

The first order spatial derivative can be approximated by the backward difference scheme if $p(x) < 0$, (otherwise, the forward difference scheme can be used if $p(x) > 0$):

$$\frac{\partial}{\partial x} p(x_1) u(x_1, t) = \frac{p(x_1) u(x_1, t) - p(x_{1-1}) u(x_{1-1}, t)}{h} + O(h). \quad (5.19)$$

The nonlinear source term can be discretised either explicitly or implicitly. In this paper, we use an explicit method and evaluate the nonlinear source term at the previous time step:

$$s(u(x, t_{n+1}), x, t_{n+1}) = s(u(x, t_n), x, t_n) + O(\tau). \quad (5.20)$$

In this way, we avoid solving a nonlinear system at each time step and obtain an unconditionally stable and convergent numerical scheme, as shown in Section 5.3. However, the shortcoming of the explicit method is that it generates additional temporal error, as shown in Eq.(5.20).
Thus, using Eqs. (5.17)-(5.20), we have

\[
\frac{\tau^{-\alpha}}{\Gamma(2 - \alpha)} \sum_{j=0}^{n} b_j [u(x_i, t_{n+1-j}) - u(x_i, t_{n-j})] = p(x_i)u(x_i, t_{n+1}) - p(x_i-1)u(x_i-1, t_{n+1})
\]

\[
- \frac{K_{\alpha} h^{1-\mu}}{2 \cos(\frac{\pi \mu}{2})} \left[ \sum_{i=0}^{l+1} w_i u(x_{i+1}, t_{n+1}) + \sum_{i=0}^{M-l+1} w_i u(x_{i+1}, t_{n+1}) \right]
\]

\[
+ s(u(x_i, t_n), x_i, t_n) + O(\tau^{1+\alpha} + h + \tau).
\]  

(5.21)

After some manipulation, Eq. (5.21) can be written in the following form:

\[
u(x_i, t_{n+1}) = b_n u(x_i, t_0) + \sum_{j=0}^{n-1} (b_j - b_{j+1}) u(x_i, t_{n-j})
\]

\[
+ \frac{\mu_0}{h} \left( p(x_i)u(x_i, t_{n+1}) - p(x_i-1)u(x_i-1, t_{n+1}) \right)
\]

\[
- \mu_0 r_0 \left[ \sum_{i=0}^{l+1} w_i u(x_{i+1}, t_{n+1}) + \sum_{i=0}^{M-l+1} w_i u(x_{i+1}, t_{n+1}) \right]
\]

\[
+ \mu_0 s(u(x_i, t_n), x_i, t_n) + R_i^{n+1},
\]

(5.22)

where \( \mu_0 = \tau^\alpha \Gamma(2 - \alpha) > 0 \), \( r_0 = \frac{K_{\alpha} h^{1-\mu}}{2 \cos(\frac{\pi \mu}{2})} < 0 \), and

\[
|R_i^{n+1}| \leq C_1 \tau^\alpha (\tau^{1+\alpha} + h + \tau).
\]

(5.23)

Let \( u_i^n \) be the numerical approximation of \( u(x_i, t_n) \); and \( s_i^n \) be the numerical approximation of \( s(u(x_i, t_n), x_i, t_n) \). We obtain the following effective numerical method (ENM) of the TSFFPE-NST (5.13)-(5.15):

\[
u_i^{n+1} = b_n u_i^0 + \sum_{j=0}^{n-1} (b_j - b_{j+1}) u_i^{n-j} + \frac{\mu_0}{h} \left( p_i u_i^{n+1} - p_{i-1} u_{i-1}^{n+1} \right)
\]

\[
- \mu_0 r_0 \left[ \sum_{i=0}^{l+1} w_i u_{i+1}^{n+1} + \sum_{i=0}^{M-l+1} w_i u_{i+1}^{n+1} \right] + \mu_0 s_i^n,
\]

(5.24)

for \( l = 1, 2, \ldots, M - 1, \ n = 0, 1, 2, \ldots, N - 1 \). The boundary and initial conditions can be
5.2 An effective numerical method for the TSFFPE-NST

discretised using

\[ u^n_0 = u^n_M = 0, \quad n = 0, 1, 2, \ldots, N, \] (5.25)

\[ u^0_l = u_0(lh), \quad l = 0, 1, 2, \ldots, M. \] (5.26)

**Remark 5.1.** If we use the implicit method to approximate the nonlinear source term, the numerical method of the TSFFPE-NST can be written as

\[ u^{n+1}_l = b_n u^0_l + \sum_{j=0}^{n-1} (b_j - b_{j+1}) u^{n-j}_l + \frac{\mu_0}{h} (p_l u^{n+1}_l - p_{l-1} u^{n+1}_{l-1}) \]

\[- \mu_0 \rho_0 \left[ \sum_{i=0}^{l+1} w_i u^{n+1}_{l+1-i} + \sum_{i=0}^{M-l+1} w_i u^{n+1}_{l+i} \right] + \mu_0 s^{n+1}_l, \] (5.27)

i.e. replace \( s^n_l \) in Eq. (5.24) with \( s^{n+1}_l \). This numerical method is stable and convergent when the source term \( s(u(x, t), x, t) \) satisfies the Lipschitz condition (5.16). (See eg. [87])

**Lemma 5.1.** [169] The coefficients \( b_j \) satisfy

1. \( b_j > 0 \) for \( j = 0, 1, 2, \ldots, n; \)

2. \( 1 = b_0 > b_1 > \ldots > b_n, b_n \to 0 \) as \( n \to \infty; \)

3. When \( 0 < \alpha < 1, \)

\[ \lim_{j \to \infty} \frac{b^{-1}_j}{j^\alpha} = \lim_{j \to \infty} \frac{j^{-1}}{(1 + j^{-1})^{1-\alpha} - 1} = \frac{1}{1 - \alpha}. \]

Thus, there is a positive constant \( C_2 \) such that

\[ b^{-1}_j \leq C_2 j^\alpha, \quad j = 0, 1, 2, \ldots. \]

**Lemma 5.2.** [106] The coefficients \( w_i \) satisfy

1. \( w_0 = 0, w_1 = -\mu < 0, \) and \( w_i > 0 \) for \( i = 2, 3, \ldots, M; \)

2. \( \sum_{i=0}^{\infty} w_i = 0, \) and \( \sum_{i=0}^{n} w_i < 0 \) for \( \forall n \in \mathbb{N}. \)
Chapter 5. Stability and convergence of an ENM for TSFFPE-NST

5.3 Stability of the effective numerical method (ENM)

In this section, we analyse the stability of the ENM (5.24)-(5.26). Firstly, we rewrite (5.24) in the following form

\[ u_{l}^{n+1} - \frac{\mu_{0}}{h} (p_{l}u_{l}^{n+1} - p_{l-1}u_{l-1}^{n+1}) + \mu_{0} r_{0} \left[ \sum_{i=0}^{l+1} w_{i} u_{l-i+1}^{n+1} + \sum_{i=0}^{M-l+1} w_{i} u_{l-i+1}^{n+1} \right] = b_{n} u_{0}^{n} + \sum_{j=0}^{n-1} (b_{j} - b_{j+1}) u_{l}^{n-j} + \mu_{0} s_{l}^{n}. \] (5.28)

Let \( \tilde{u}_{l}^{n} \) be the approximate solution of the ENM (5.28); \( \tilde{s}_{l}^{n} \) be the approximation of \( s_{l}^{n} \). Setting \( \rho_{l}^{n} = u_{l}^{n} - \tilde{u}_{l}^{n} \), we obtain the following roundoff error equation:

\[ \rho_{l}^{n+1} - \frac{\mu_{0}}{h} (p_{l}\rho_{l}^{n+1} - p_{l-1}\rho_{l-1}^{n+1}) + \mu_{0} r_{0} \left[ \sum_{i=0}^{l+1} w_{i} \rho_{l-i+1}^{n+1} + \sum_{i=0}^{M-l+1} w_{i} \rho_{l-i+1}^{n+1} \right] = b_{n} \rho_{0}^{n} + \sum_{j=0}^{n-1} (b_{j} - b_{j+1}) \rho_{l}^{n-j} + \mu_{0} (s_{l}^{n} - \tilde{s}_{l}^{n}), \] (5.29)

for \( l = 1, 2, \ldots, M - 1; \ n = 0, 1, \ldots, N - 1 \).

We suppose that \( p(x) \leq 0 \) and that \( p(x) \) decreases monotonically on \([a, b]\). This is based on the fact that physical considerations and stability dictate that \( p'(x) < 0 \) [28, 122]. Assuming \( \|\rho^{n}\|_{\infty} = \max_{1 \leq l \leq M-1} |\rho_{l}^{n}| \), and using mathematical induction, we obtain the following theorem.

**Theorem 5.1.** Suppose that \( \rho_{l}^{n} \ (l = 1, 2, \ldots, M - 1; \ n = 1, 2, \ldots, N) \) is the solution of the roundoff error equation (5.29), and the nonlinear source term \( s(u(x, t), x, t) \) satisfies the Lipschitz condition (5.16), then there is a positive constant \( C_{0} \), such that

\[ \|\rho^{n}\|_{\infty} \leq C_{0} \|\rho^{0}\|_{\infty}, \quad n = 1, 2, \ldots, N. \]

**Proof.** When \( n = 1 \), assume that \( |\rho_{0}^{1}| = \max\{|\rho_{1}^{1}|, |\rho_{2}^{1}|, \ldots, |\rho_{M-1}^{1}|\} \). Because \( p(x) \leq 0 \) and decreases monotonically on \([a, b]\), we have

\[ 0 \leq -\frac{\mu_{0}}{h} (p_{0} - p_{0-1})|\rho_{0}^{1}| \leq -\frac{\mu_{0}}{h} p_{0}|\rho_{0}^{1}| + \frac{\mu_{0}}{h} p_{0-1}|\rho_{0-1}^{1}|. \] (5.30)

5.3 Stability of the effective numerical method (ENM)

Using the properties of $\omega_i$ in Lemma 5.2, we have

\[
0 \leq \mu_0 r_0 \left[ \sum_{i=0}^{l_0+1} w_i |\rho_{i_0}^1| + \sum_{i=0}^{M-l_0+1} w_i |\rho_{i_0}^1| \right] \\
\leq \mu_0 r_0 \left[ \sum_{i=0}^{l_0+1} w_i |\rho_{i_0-i+1}^1| + \sum_{i=0}^{M-l_0+1} w_i |\rho_{i_0+i-1}^1| \right]. \tag{5.31}
\]

Combining (5.30) with (5.31), using the Lipschitz condition (5.16) and smooth solution condition, we obtain

\[
|\rho_{l_0}^1| \leq |\rho_{l_0}^1| - \frac{\mu_0}{h} |p_{l_0}| - \frac{\mu_0}{h} |p_{l_0-1}| \\
+ \mu_0 r_0 \left[ \sum_{i=0}^{l_0+1} w_i |\rho_{i_0-i+1}^1| + \sum_{i=0}^{M-l_0+1} w_i |\rho_{i_0+i-1}^1| \right] \\
\leq |b_0 \rho_{l_0}^0 + \mu_0 (s_{l_0}^0 - \tilde{s}_{l_0}^0)| \\
\leq b_0 |\rho_{l_0}^0| + \mu_0 L |\rho_{l_0}^0| = (1 + \mu_0 L) |\rho_{l_0}^0|. \tag{5.32}
\]

Let $C = 1 + \mu_0 L$. Thus, we obtain

\[
\|\rho^1\|_\infty \leq C \|\rho^0\|_\infty. \tag{5.33}
\]

Now, suppose that

\[
\|\rho^k\|_\infty \leq C \|\rho^0\|_\infty, \quad k = 2, \ldots, n. \tag{5.34}
\]
By assuming $|ρ^{n+1}_0| = \max\{|ρ^{n+1}_1|, |ρ^{n+1}_2|, \ldots, |ρ^{n+1}_{M-1}|\}$, we have that

$$
|ρ^{n+1}_0| \leq \rho^{n+1}_0 - \frac{μ_0}{h} \left( p_0 ρ^{n+1}_0 - p_0 \rho^{n+1}_0 \right) + \mu_0 r_0 \sum_{i=0}^{l_0+1} w_i ρ^{n+1}_{l_0-i+1} + \sum_{i=0}^{M-l_0+1} w_i ρ^{n+1}_{l_0+i-1}
$$

$$
= b_n ρ^0_0 + \sum_{j=0}^{n-1} (b_j - b_{j+1}) ρ^{n-j}_0 + \mu_0 (s^0_{l_0} - \tilde{s}_{l_0}^0)
$$

$$
\leq b_n |ρ^0_0| + \sum_{j=0}^{n-1} (b_j - b_{j+1}) |ρ^{n-j}_0| + \mu_0 L |ρ^0_0|.
$$

(5.35)

Using (5.33) and (5.34), we have

$$
|ρ^{n+1}_0| \leq b_n |ρ^0_0| + C \sum_{j=0}^{n-1} (b_j - b_{j+1}) |ρ^0_0| + C μ_0 L |ρ^0_0|
$$

$$
= b_n |ρ^0_0| + C (b_0 - b_n) |ρ^0_0| + C μ_0 L |ρ^0_0|
$$

$$
= (b_n μ_0 L + C^2) |ρ^0_0|.
$$

(5.36)

Let $C_0 = b_n μ_0 L + C^2$. Hence, we have

$$
||ρ^{n+1}||_{∞} \leq C_0 ||ρ^0||_{∞}.
$$

(5.37)

The proof of Theorem 5.1 is completed.

Applying Theorem 5.1, the following theorem of stability is obtained.

**Theorem 5.2.** Assuming the nonlinear source term $s(u(x,t), x, t)$ satisfies the Lipschitz condition (5.16), and that the drift coefficient $p(x) \leq 0$ decreases monotonically on $[a, b]$, the ENM defined by (5.24)-(5.26) is stable.

**Remark 5.2.** If $p(x) > 0$ and decreases monotonically on $[a, b]$, we can use the forward difference method to approximate the first order spatial derivative, and apply a similar analysis of stability.

**Remark 5.3.** In fact, for the case $p(x)$ does not decrease monotonically, we can still obtain a stable numerical scheme by a minor change in our current ENM. We can expand the first term on the RHS of Eq.(5.13) as $\frac{∂}{∂x}[p(x)u(x,t)] = \frac{∂p}{∂x}u(x,t) + p(x)\frac{∂u(x,t)}{∂x}$, which enables us to group $\frac{∂p}{∂x}u(x,t)$ together with the nonlinear source term $s(u, x, t)$ to obtain a new nonlinear
source term \( s^*(u, x, t) = s(u, x, t) + \frac{dp}{dx} u(x, t) \). This way we can weaken the assumption on \( p(x) \) and the analysis given in this section still can be used.

**Remark 5.4.** If we use an implicit method to approximate the nonlinear source term, as shown in Remark 5.1, we can prove that the numerical method defined in Eq.(5.27) is stable when \( 1 - \mu_0L > 0 \), which is independent of the spatial step. In fact, when the time step is small, the condition \( 1 - \mu_0L > 0 \) is generally satisfied.

### 5.4 Convergence of the effective numerical method (ENM)

In this section, we analyse the convergence of the ENM (5.24)-(5.26). Let \( u(x_l, t_n) \) be the exact solution of the TSFFPE-NST (5.13)-(5.15) at mesh point \((x_l, t_n)\), and \( u^n_l \) be the numerical solution of the TSFFPE-NST (5.13)-(5.15) computed using the ENM (5.24)-(5.26). Define \( \eta^n_l = u(x_l, t_n) - u^n_l \) and \( Y^n = (\eta^n_0, \eta^n_1, \ldots, \eta^n_{M-1})^T \). Subtracting (5.24) from (5.22) leads to

\[
\eta^{n+1}_l = \frac{\mu_0}{\beta} \left( p_l \eta^{n+1}_l - p_{l-1} \eta^{n+1}_{l-1} \right) + \mu_0 r_0 \left[ \sum_{i=0}^{l+1} w_i \eta^{n+1}_{i-1} + \sum_{i=0}^{M-l+1} w_i \eta^{n+1}_{i+1} \right] \\
= b^n_l \eta^n_0 + \sum_{j=0}^{n-1} (b_j - b_{j+1}) \eta^{n-j}_l + \mu_0 \left( s(u(x_l, t_n), x_l, t_n) - s^n_l \right) + R^{n+1}_l, \quad (5.38)
\]

where \( l = 1, 2, \ldots, M - 1; \ n = 0, 1, \ldots, N - 1. \)

Assuming \( \|Y^n\|_{\infty} = \max_{1 \leq l \leq M-1} |\eta^n_l| \) and using mathematical induction, we obtain the following theorem.

**Theorem 5.3.** Assuming the nonlinear source term \( s(u(x, t), x, t) \) satisfies the Lipschitz condition (5.16), and the drift coefficient \( p(x) \leq 0 \) decreases monotonically on \([a, b]\), the ENM defined by (5.24)-(5.26) is convergent, and there exists a positive constant \( C^* \), such that

\[
\|Y^n\|_{\infty} \leq C^*(\tau^{1+\alpha} + h + \tau), \quad n = 1, 2, \ldots, N. \quad (5.39)
\]

**Proof.** Assume \( |R^{k_0}_{l_0}| = \max_{1 \leq l \leq M-1, 1 \leq n \leq N} |R^n_l| \). Following a similar argument to that presented above for the stability analysis of the ENM (5.24)-(5.26), when \( n = 1 \), assuming that \( |\eta^n_{l_0}| = \ldots \)
max\{|\eta_1^1|, |\eta_2^1|, \ldots, |\eta^{M-1}_1|\}, we have

\[
|\eta^1_{l_0}| \leq |b_0\eta^0_{l_0} + \mu_0(s(u(x_{l_0}, t_0), x_{l_0}, t_0) - s^0_{l_0}) + R^1_{l_0}|.
\] (5.40)

Utilising \(Y^0 = 0\), the Lipschitz condition (5.16) and smooth solution condition, we obtain

\[
|\eta^1_{l_0}| \leq b_0|\eta^0_{l_0}| + \mu_0 L|\eta^0_{l_0}| + |R^k_{l_0}| = |R^k_{l_0}|.
\] (5.41)

Thus,

\[
\|Y^1\|_\infty \leq |R^k_{l_0}|.
\] (5.42)

Now, suppose that

\[
\|Y^k\|_\infty \leq b^{-1}_{k-1}|R^k_{l_0}|, \quad k = 1, 2, \ldots, n.
\] (5.43)

Using Lemma 5.2, \(b_k > b_{k+1}\), we have

\[
\|Y^k\|_\infty \leq b^{-1}_{n}|R^k_{l_0}|.
\] (5.44)

Similarly, assuming \(|\eta^{n+1}_{l_0}| = \max\{|\eta^{n+1}_1|, |\eta^{n+1}_2|, \ldots, |\eta^{n+1}_{M-1}|\}\), we have

\[
|\eta^{n+1}_{l_0}| \leq b_n|\eta^0_{l_0}| + \sum_{j=0}^{n-1} (b_j - b_{j+1}) |\eta^{n-j}_{l_0}| + \mu_0(s(u(x_{l_0}, t_n), x_{l_0}, t_n) - s^0_{l_0}) + R^{n+1}_{l_0}|
\] (5.45)

Utilising \(Y^0 = 0\), the Lipschitz condition (5.16) and smooth solution condition, we obtain

\[
|\eta^{n+1}_{l_0}| \leq b^{-1}_n(b_0 - b_n)|R^k_{l_0}| + \mu_0 L b^{-1}_n |R^k_{l_0}| + |R^k_{l_0}|
\]

\[
= b^{-1}_n(b_0 - b_n + \mu_0 L + b_n)|R^k_{l_0}|
\]

\[
= b^{-1}_n(b_0 + \mu_0 L)|R^k_{l_0}| = C b^{-1}_n |R^k_{l_0}|.
\] (5.46)

Hence,

\[
\|Y^{n+1}\|_\infty \leq C b^{-1}_n |R^k_{l_0}|.
\]

Finally, utilising (5.23) and Lemma 5.1, \(b^{-1}_n \leq C_2 n^\alpha\), we obtain the result on the convergence
5.5 Numerical results

of the ENM (5.24)-(5.26), namely

\[ \|Y^n\|_\infty \leq CC_1C_2^n\tau^\alpha (\tau^{1+\alpha} + h + \tau) \leq C^\ast (\tau^{1+\alpha} + h + \tau), \]

(5.47)

for \( n = 1, 2, \ldots, N \).

Remark 5.5. If we use an implicit method to approximate the nonlinear source term, as shown in Remark 5.1, we can prove that the numerical method defined in Eq. (5.27) is convergent when \( 1 - \mu_0L > 0 \), which is independent of the spatial step. In fact, when the time step is small, the condition \( 1 - \mu_0L > 0 \) is generally satisfied.

5.5 Numerical results

In this section, we present four numerical examples of the TSFFPE to demonstrate the accuracy of our theoretical analysis. We also use our solution method to illustrate the changes in solution behaviour that arise when the exponent is varied from integer order to fractional order, and to identify the differences between solutions with and without the external force term.

Example 5.1. Consider the following TSFFPE:

\[
\begin{align*}
\frac{\partial^\alpha u(x, t)}{\partial t^\alpha} & = \left[ -\upsilon \frac{\partial}{\partial x} + K^\alpha \mu \frac{\partial^\mu}{\partial|x|^\mu} \right] u(x, t) + f(x, t), \\
u(a, t) & = u(b, t) = 0, \quad 0 \leq t \leq T, \\
u(x, 0) & = K^\mu \alpha (x - a)^2(b - x)^2, \quad a \leq x \leq b,
\end{align*}
\]

(5.49)

where

\[
f(x, t) = (1 + \alpha)\upsilon \Gamma(1 + \alpha)t(x - a)^2(b - x)^2 \\
+ \frac{K^\mu \alpha (K^\mu \alpha + \upsilon t^{1+\alpha})}{2 \cos\left(\frac{\pi \mu}{2}\right)} [g(x - a) + g(b - x)] \\
+ 2\upsilon (K^\alpha \mu + \upsilon t^{1+\alpha})(x - a)(b - x)(a + b - 2x),
\]

\[
g(x) = \frac{4!}{\Gamma(5 - \mu)}x^{3-\mu} - 2(b - a)\frac{3!}{\Gamma(4 - \mu)}x^{2-\mu} \\
+ (b - a)^2\frac{2}{\Gamma(3 - \mu)}x^{2-\mu}.
\]
Figure 5.1: Comparison of the numerical solution with the exact solution for Example 5.1 at $T = 1.0, 3.0, 5.0$. $T$ increases in the direction of the arrow.

Table 5.1: Maximum error behaviour versus grid size reduction for Example 5.1 at $T = 1.0$.

<table>
<thead>
<tr>
<th>$h = \tau$</th>
<th>Maximum error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/10</td>
<td>4.8148E-2</td>
</tr>
<tr>
<td>1/20</td>
<td>1.0111E-2</td>
</tr>
<tr>
<td>1/40</td>
<td>2.0587E-3</td>
</tr>
<tr>
<td>1/80</td>
<td>7.3019E-4</td>
</tr>
</tbody>
</table>

The exact solution of the TSFFPE (5.48)-(5.50) is found to be

$$u(x,t) = (K^{\mu}_a + \nu t^{1+\alpha})(x-a)^2(b-x)^2,$$

which can be verified by direct fractional differentiation of the given solution, and substituting into the fractional differential equation.

In this example, we take $a = 0$, $b = 1$, $K^{\mu}_a = 25$, $\nu = 1$, $\alpha = 0.8$, $\mu = 1.9$. From Figure 5.1, it can be seen that the numerical solution using the ENM is in good agreement with the exact solution at different times $T$, with $h = 1/40$ and $\tau = 1/100$. The maximum errors of the ENM at time $T = 1.0$ are presented in Table 5.1. It can be seen that the ENM is stable and convergent for solving the TSFFPE (5.48)-(5.50). The errors, as our theory indicated, satisfy the relationship $\text{error} \leq (\tau^{1+\alpha} + h + \tau)$.
Example 5.2. Consider the following TSFFPE-NST

\[
\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = K^\mu_\alpha \frac{\partial^\mu}{\partial |x|^\mu} u(x,t) - \frac{\gamma}{\Gamma(\beta)} \int_0^t (t - \xi)^{\beta-1} u(x, \xi) d\xi, \tag{5.52}
\]

\[
u(-5,t) = u(5,t) = 0, \quad 0 \leq t \leq T, \tag{5.53}
\]

\[
u(x,0) = \delta(x). \tag{5.54}
\]

This example is a TSFFPE-NST without the external force term. In fact, it reduces to the fractional diffusion equation with an absorbent term. The formulae to approximate the absorbent term is presented in Appendix 5.7. Here, we take \(\beta = 0.5\), \(\gamma = 1\), and \(K^\mu_\alpha = 1\). Figures 5.2-5.4 show the changes in the solution profiles of the TSFFPE-NST (5.52)-(5.54) when \(\alpha\) and \(\mu\) are changed from integer to fraction at different times \(T\). We see that the solution profile of the fractional order model is characterised by a sharp peak and a heavy tail. The peak height in Figure 5.2 (\(\alpha = 1.0\) and \(\mu = 2.0\)) decreases more rapidly than that in Figure 5.3 (\(\alpha = 0.8\), and \(\mu = 1.8\)). Furthermore, when we choose \(\alpha = 0.5\) and \(\mu = 1.5\), a more interesting result can be observed, that is, the peak height in Figure 5.2 decreases more slowly than that shown in Figure 5.4 at the early time \(T = 0.1\), but this trend reverses for the later times \(T = 0.5\) and \(T = 1.0\). Hence, the TSFFPE-NST (5.52)-(5.54) may be useful to investigate several physical processes in the absence of an external force field by choosing appropriate \(\alpha\) and \(\mu\).
Figure 5.3: Numerical solutions for Example 5.2 with $\alpha = 0.8$ and $\mu = 1.8$ at different times $T = 0.1, 0.5, 1.0$.

Figure 5.4: Numerical solutions for Example 5.2 with $\alpha = 0.5$ and $\mu = 1.5$ at different times $T = 0.1, 0.5, 1.0$. 
Example 5.3. Consider the following TSFFPE-NST

\[
\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \left[ \frac{\partial}{\partial x} p(x) + K_\alpha^\mu \frac{\partial^\mu}{\partial |x|^\mu} \right] u(x,t) - \frac{\gamma}{\Gamma(\beta)} \int_0^t (t - \xi)^{\beta-1} u(x,\xi) d\xi, \hspace{1cm} (5.55)
\]

\[
u(-5,t) = u(5,t) = 0, \hspace{1cm} 0 \leq t \leq T, \hspace{1cm} (5.56)
\]

\[
u(x,0) = \delta(x). \hspace{1cm} (5.57)
\]

This example of the TSFFPE-NST incorporates the external force term with \( p(x) = -1 \) and an absorbent term. The formula to approximate the absorbent term is presented in Appendix 5.7. Here, we take \( \beta = 0.5, \gamma = 1, \) and \( K_\alpha^\mu = 1. \) Figures 5.5-5.7 show the changes in the solution profiles of the TSFFPE-NST (5.55)-(5.57) when \( \alpha \) and \( \mu \) are changed from integer order to fractional order at different times \( T. \) Again, we see that the solution profile of the fractional order model is characterised by a sharp peak and a heavy tail. Furthermore, due to the presence of the external force term with \( p(x) = -1, \) the solution profiles are shifted to the right. It is worthwhile to note that the peak of the integer order model in Figure 5.5 (\( \alpha = 1.0 \) and \( \mu = 2.0 \)) moves to the right as time increases, but the peak of the fractional order model in Figure 5.6 (\( \alpha = 0.8, \) and \( \mu = 1.8 \)) and Figure 5.7 (\( \alpha = 0.5 \) and \( \mu = 1.5 \)) does not move.

We also see that the peak heights in Figure 5.5 and Figure 5.6 remain almost the same for increasing time. The peak height in Figure 5.5 decreases more slowly than that shown in Figure 5.7 at the early time \( T = 0.1, \) but this trend reverses for the later times \( T = 0.5 \) and \( T = 1.0. \) Hence, the TSFFPE-NST (5.55)-(5.57) may be useful to investigate several physical processes within an external force field by choosing appropriate \( \alpha \) and \( \mu. \)

Example 5.4. Consider the following TSFFPE-NST

\[
\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \left[ \frac{\partial}{\partial x} p(x) + K_\alpha^\mu \frac{\partial^\mu}{\partial |x|^\mu} \right] u(x,t) + ru(x,t) \left( 1 - \frac{u(x,t)}{K} \right), \hspace{1cm} (5.58)
\]

\[
u(0,0) = u(5,0) = 0, \hspace{1cm} 0 \leq t \leq T, \hspace{1cm} (5.59)
\]

\[
u(x,0) = x^2(5 - x)^2, \hspace{1cm} 0 \leq x \leq 5. \hspace{1cm} (5.60)
\]

In applications to population biology, \( u(x,t) \) is the population density at location \( x \in \mathbb{R} \) and time \( t > 0. \) The nonlinear source term \( s(u(x,t), x, t) = ru(x,t)(1 - u(x,t)/K) \) is the Fisher’s growth term that models population growth, where \( r \) is the intrinsic growth rate of a
Figure 5.5: Numerical solutions for Example 5.3 with $\alpha = 1.0$ and $\mu = 2.0$ at different times $T = 0.1, 0.5, 1.0$.

Figure 5.6: Numerical solutions for Example 5.3 with $\alpha = 0.8$ and $\mu = 1.8$ at different times $T = 0.1, 0.5, 1.0$. 
Figure 5.7: Numerical solutions for Example 5.3 with $\alpha = 0.5$ and $\mu = 1.5$ at different times $T = 0.1, 0.5, 1.0$.

species and $K$ is the environmental carrying capacity, representing the maximum sustainable population density [9, 27, 98].

In this example, we take $r = 0.2$, $K = 1$. Figure 5.8 shows the solution behaviour when $\alpha = 0.8$, $\mu = 1.6$ at different times $T = 0.1, 0.5, 1.0$, while Figure 5.9 shows the solution behaviour with different values of $\alpha$ between 0 and 1, and fixed value of $\mu = 1.8$ at time $T = 1.0$. Figure 5.9 also shows that the system exhibits anomalous diffusion behaviour and that the solution continuously depends on the time and space fractional derivatives. Although the source term for the Fisher’s equation $s(u(x,t),x,t) = ru(x,t)(1 - u(x,t)/K)$ is not globally Lipschitz continuous, the solution of the discrete numerical method still yields bounds on the solution of the continuous problem and the solution of the numerical method (ENM) converges to the unique solution of the continuous problem (5.58)-(5.60) as the time and space steps tend to zero [8].

5.6 Conclusions

In this paper, we have proposed an effective numerical method to solve the TSFFPE-NST and proved that the ENM is stable and convergent provided that the nonlinear source term satisfies the Lipschitz condition, the solution of the continuous problem satisfies the smooth solution
Figure 5.8: Numerical solutions for Example 5.4 with $\alpha = 0.8$ and $\mu = 1.6$ at different times $T = 0.1, 0.5, 1.0$.

Figure 5.9: Numerical solutions for Example 5.4 with fixed $\mu = 1.8$ at time $T = 1.0$, and different values of $\alpha = 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$. 
condition, and $p'(x)$ can be either $> 0$ or $< 0$. Numerical experiments have been carried out to support the theoretical claims. These numerical methods can also be used to investigate other types of fractional partial differential equations.

5.7 Appendix: Formulae for Examples 5.2 and 5.3

Let us start from Eq. (5.28), i.e.

$$
u_{l+1}^{n+1} = \frac{\mu_0}{h} (p_l u_l^{n+1} - p_{l-1} u_{l-1}^{n+1}) + \mu_0 r_0 \left[ \sum_{i=0}^{l+1} w_i u_i^{n+1} + \sum_{i=0}^{M-l+1} w_i u_i^{n+1} \right]$$

$$= b_n u_l^0 + \sum_{j=0}^{n-1} (b_j - b_{j+1}) u_l^{n-j} + \mu_0 s_l^n. \quad (5.61)$$

Now setting $s_l^n = -\frac{\gamma}{\Gamma(\beta)} \int_{0}^{t_n} (t_n - \xi)^{\beta-1} u(x_l, \xi) d\xi$, then we have

$$s_l^n \approx -\frac{\gamma}{\Gamma(\beta)} \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} (t_n - \xi)^{\beta-1} u(x_l, \xi) d\xi. \quad (5.62)$$

Applying the Mean Value Theorem (M.V.T) for integration yields

$$s_l^n \approx -\frac{\gamma}{\Gamma(\beta)} \sum_{j=0}^{n-1} u_l^j + u_l^{j+1} \left[ \frac{(t_n - t_j)^\beta}{\beta} - \frac{(t_n - t_{j+1})^\beta}{\beta} \right]$$

$$= -\frac{\gamma \tau}{\Gamma(\beta) \cdot 2 \cdot \beta} \sum_{j=0}^{n-1} (u_l^j + u_l^{j+1}) \left[ (n-j)^\beta - (n-j-1)^\beta \right]$$

$$= -\frac{\gamma \tau}{2\Gamma(\beta + 1)} \sum_{j=0}^{n-1} (u_l^{n-j-1} + u_l^{n-j}) \left[ (j+1)^\beta - j^\beta \right]$$

$$= -\mu_1 \sum_{j=0}^{n-1} q_j (u_l^{n-j-1} + u_l^{n-j}), \quad (5.63)$$

where $\mu_1 = \frac{\gamma \tau}{2\Gamma(\beta + 1)}$, $q_j = (j+1)^\beta - j^\beta$, $j = 0, 1, \ldots$. 


Also, we have
\[
\sum_{i=0}^{l+1} w_i u_{l-i+1}^{n+1} + \sum_{i=0}^{M-l+1} w_i u_{l+i-1}^{n+1} = \sum_{i=0}^{M-1} \eta_i u_i^{n+1},
\tag{5.64}
\]
where
\[
\eta_i = \begin{cases} 
  u_{l-i+1}, & 1 \leq i \leq l - 2, \\
  w_0 + w_2, & i = l - 1, \\
  2w_1, & i = l, \\
  w_0 + w_2, & i = l + 1, \\
  w_{i-l+1}, & l + 2 \leq i \leq M - 1,
\end{cases}
\tag{5.65}
\]

Now, substituting (5.63) and (5.64) into (5.61), we obtain the numerical scheme for Example 5.2 as
\[
u_{l+1}^{n+1} + \mu_0 r_0 \sum_{i=0}^{M-1} \eta_i u_i^{n+1} = b_n u_0^l + \sum_{j=0}^{n-1} \left[ (b_j - b_{j+1}) u_{l+1}^{n-j} - \mu_1 q_j (u_i^{n-j-1} + u_i^{n-j}) \right],
\tag{5.66}
\]
and the numerical scheme for Example 5.3 as
\[
(1 - \frac{\mu_0 \mu_1}{h}) u_{l+1}^{n+1} + \frac{\mu_0 \mu_i}{h} u_{l-1}^{n+1} + \mu_0 r_0 \sum_{i=0}^{M-1} \eta_i u_i^{n+1} = b_n u_0^l + \sum_{j=0}^{n-1} \left[ (b_j - b_{j+1}) u_{l+1}^{n-j} - \mu_1 q_j (u_i^{n-j-1} + u_i^{n-j}) \right].
\tag{5.67}
\]
CHAPTER 6

Two new implicit numerical methods for the fractional cable equation

6.1 Introduction

During the past three decades, the concept of fractional calculus (that is, calculus of integrals and derivatives of any arbitrary real or complex order) has gained considerable popularity and importance, due to its demonstrated applications in numerous seemingly diverse and widespread fields of science, engineering, and finance. For example, fractional calculus has been successfully applied to problems in system biology [159], physics [11, 108, 110, 128, 160], chemistry and biochemistry [156], hydrology [13, 14, 78, 79], medicine [54, 99], and finance [51, 120, 132, 148].

The cable equation is one of the most fundamental equations for modelling neuronal dynamics. The Nernst-Planck equation of electrodifussion for the movement of ions in neurons has also been shown to be equivalent to the cable equation under simplifying assumptions [119]. Some authors have elucidated that if the ions are undergoing anomalous subdiffusion then the comparison with models that assume standard or normal diffusion will likely lead to incorrect or
misleading diffusion coefficient values [131] and models that incorporate anomalous diffusion should be used. Langlands et al. [69, 70] derived a fractional variant of the Nernst-Planck equation to model the anomalous subdiffusion of the ions.

A recent study on spiny Purkinje cell dendrites showed that spines trap and release diffusing molecules resulting in anomalously slow molecular diffusion along the dendrite [130]. The diffusive spatial variance \( \langle r^2(t) \rangle \) of an inert tracer was found to evolve as a sublinear power law in time, i.e., \( \langle r^2(t) \rangle \sim t^\gamma \) with \( 0 < \gamma < 1 \). The diffusion became more anomalous (smaller \( \gamma \)) with increasing spine density. Henry et al. [54] derived a fractional cable equation from the fractional Nernst-Planck equations to model anomalous electrodiffusion of ions in spiny dendrites. They subsequently found a fractional cable equation by treating the neuron and its membrane as two separate materials governed by separate fractional Nernst-Planck equations and employed a small ionic concentration gradient assumption [69, 70]. The resulting equation involves two fractional temporal Riemann-Liouville derivatives.

In this paper, we consider the following initial-boundary value problem of the fractional cable equation:

\[
\frac{\partial u(x, t)}{\partial t} = 0D^{1-\gamma_1}_t \left( K \frac{\partial^2 u(x, t)}{\partial x^2} \right) - \mu^2 0D^{1-\gamma_2}_t u(x, t) + f(x, t), \quad (6.1)
\]

\[
u(x, 0) = g(x), \quad 0 \leq x \leq L, \quad (6.2)
\]

\[
u(0, t) = \varphi(t), \quad u(L, t) = \psi(t), \quad 0 \leq t \leq T, \quad (6.3)
\]

where \( 0 < \gamma_1, \gamma_2 < 1 \), \( K > 0 \) and \( \mu \) are constants, and \( 0D^{1-\gamma}_t u(x, t) \) is the Riemann-Liouville fractional partial derivative of order \( 1 - \gamma \) defined by

\[
0D^{1-\gamma}_t u(x, t) = \frac{1}{\Gamma(\gamma)} \frac{\partial}{\partial t} \int_0^t \frac{u(x, \eta)}{(t-\eta)^{1-\gamma}} d\eta = \frac{\partial}{\partial t} I^{\gamma}_0 u(x, t), \quad (6.4)
\]

where \( I^{\gamma}_0 y(t) = \frac{1}{\Gamma(\gamma)} \int_0^t \frac{y(\eta)}{(t-\eta)^{1-\gamma}} d\eta \) is the the Riemann-Liouville fractional integral of order \( \gamma > 0 \).

Some different numerical methods for solving space or time fractional partial differential equations have been proposed. Liu et al. [78] proposed a computationally effective method of
lines. This method transforms the space fractional partial differential equation into a system of ordinary differential equations that is then solved using backward difference formulas. Meerschaert and Tadjeran [106] developed finite difference approximations for fractional advection-dispersion flow equations. Roop [122] investigated the computational aspects of the Galerkin approximation using continuous piecewise polynomial basis functions on a regular triangulation of the bounded domain in $\mathbb{R}^2$. Lin and Liu [74] proposed the high order (2-6) approximations of the fractional ordinary differential equation and discussed the consistency, convergence and stability of these fractional high order methods. Liu et al. [91] discussed an approximation of the Lévy-Feller advection-dispersion process by a random walk and finite difference method. Zhuang et al. [167] proposed explicit and implicit approximations for a variable-order fractional advection-diffusion equation with a source term and discussed the stability and convergence of the methods. Lin et al. [75] also proposed a new explicit finite-difference approximation for the variable-order nonlinear fractional diffusion equation and investigated the stability and convergence of this method. Yu et al. [154] developed a reliable algorithm of the Adomian decomposition method to solve the linear and nonlinear space-time fractional reaction-diffusion equations in the form of a rapidly convergent series with easily computable components, but did not give its theoretical analysis. Some researchers have found that it is a more difficult task to solve the anomalous subdiffusion equation, which involves an integro-differential equation.

Yuste and Acedo [158] proposed an explicit finite difference method and a new von Neumann-type stability analysis for the anomalous subdiffusion equation (6.1) with $\mu = 0$. Yuste [157] also proposed weighted average finite difference methods for this equation. However they did not give a convergence analysis and pointed out the difficulty of this task when implicit methods are considered. Langlands and Henry [71] also investigated this problem and proposed an implicit numerical scheme $L_1$ approximation, and discussed the accuracy and stability of this scheme. However, the global accuracy of the implicit numerical scheme has not been derived and it seems that the unconditional stability for all $\gamma$ in the range $0 < \gamma \leq 1$ has not been established. Recently, Chen and Liu et al. presented a Fourier method for the anomalous subdiffusion equation [22] and Stokes’ first problem for a heated generalised second grade fluid with a fractional derivative [20], and they gave the stability analysis and the global accuracy analysis of the difference approximation scheme. Zhuang and Liu et al. [166] also proposed
new solution and analytical techniques of implicit numerical methods for the anomalous sub-diffusion equation that only involves one fractional temporal derivative in the diffusion term. Liu et al. [87] considered both numerical and analytical techniques for the modified anomalous subdiffusion equation with a nonlinear source term. However, computationally effective implicit numerical methods and analytical techniques for solving the fractional cable equation are still in their infancy.

The main purpose of this paper is to solve and analyse this problem by introducing numerical and analytical techniques. One contribution of this paper is that we propose two new implicit numerical methods for the fractional cable equation, which involves two integro-differential equations. The two implicit numerical methods in this paper are different from [166], due to the fractional cable equation involving a reaction term. Another contribution of this paper is that we introduce two new energy forms, together with new techniques for the stability and convergence analysis. Because the fractional cable equation involves two integro-differential equations, its stability and convergence analysis become more perplexing to handle. Some numerical examples are presented to demonstrate the effectiveness of both implicit numerical methods. These techniques can also be applied to solve other types of partial differential equations that involve several integro-differential equations. Finally, the numerical techniques presented have enabled the case $\gamma_1 \neq \gamma_2$ to be simulated, which we believe is another new contribution to the literature.

The structure of the remainder of this paper is as follows. In Section 6.2, a new implicit numerical method with convergence order $O(\tau + h^2)$ for the fractional cable equation is proposed. In Sections 6.3 and 6.4, the stability and convergence of the numerical method with convergence order $O(\tau + h^2)$ are discussed, respectively. An improved implicit numerical method, i.e., with convergence order $O(\tau^2 + h^2)$, is also derived for the fractional cable equation in Section 6.5. Numerical results for solving the fractional cable equation are given in Section 6.6 to demonstrate the effectiveness of both the implicit numerical methods. Finally, some conclusions are drawn in Section 6.7.
6.2 A new implicit numerical method for the fractional cable equation

In this section we propose a new implicit numerical method for the initial-boundary value problem of the fractional cable equation.

Let $t = t_k = k\tau, \quad (k = 0, 1, \ldots, n)$ and $x = x_j = jh, \quad (j = 0, 1, \ldots, m)$, where $\tau = T/n$ and $h = L/m$ are time and space step sizes, respectively.

We introduce the following numerical approximations

$$
\frac{\partial^2 u(x_i, t)}{\partial x^2} = \frac{1}{h^2} [u(x_{i+1}, t) - 2u(x_i, t) + u(x_{i-1}, t)] - \frac{h^2}{12} \frac{\partial^4 u(x_i, t)}{\partial x^4} - \frac{h^2}{12} \frac{\partial^4 u(\xi_i, t)}{\partial x^4}, \quad x_{i-1} < \xi_i < x_{i+1},
$$

and

$$
I_0^\gamma y(t_k) = \frac{1}{\Gamma(\gamma)} \int_0^{t_k} \frac{y(\eta)}{(t_k - \eta)^{1-\gamma}} d\eta,
$$

$$
= \frac{1}{\Gamma(\gamma)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{y(\eta)}{(t_k - \eta)^{1-\gamma}} d\eta,
$$

$$
= \frac{1}{\Gamma(\gamma)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{y(t_{j+1}) + y'(\eta_j)(\eta - t_{j+1})}{(t_k - \eta)^{1-\gamma}} d\eta,
$$

$$
= \frac{\tau^\gamma}{\Gamma(\gamma + 1)} \sum_{j=0}^{k-1} b_j^{(\gamma)} y(t_{k-j}) + C k^{\gamma} \tau^{1+\gamma} \max_{0 \leq t \leq T} |y'(t)|, \quad t_j < \eta_j < t_{j+1},
$$

where $b_j^{(\gamma)} = (j + 1)^\gamma - j^\gamma, j = 0, 1, \ldots, n - 1$.

Thus, we have

**Lemma 6.1.** If $y(t) \in C^1[0, T]$, then

$$
I_0^\gamma y(t_k) = \frac{\tau^\gamma}{\Gamma(\gamma + 1)} \sum_{j=0}^{k-1} b_j^{(\gamma)} y(t_{k-j}) + R_k^\gamma,
$$

where $|R_k^\gamma| \leq C t_k^{\gamma} \tau$.

**Lemma 6.2.** [166] The coefficients $b_k^{(\gamma)} (k = 0, 1, 2, \ldots)$ satisfy the following properties:

(i) $b_0^{(\gamma)} = 1$, $b_k^{(\gamma)} > 0$, $k = 0, 1, 2, \ldots$;
(ii) \( b_k^{(\gamma)} > b_{k+1}^{(\gamma)} \), \( k = 0, 1, 2, \ldots \);

(iii) There exists a positive constant \( C > 0 \), such that \( \tau \leq C b_k^{(\gamma)} \tau^\gamma \), \( k = 1, 2, \ldots \).

(iv) \( \sum_{j=0}^{k} b_j^{(\gamma)} \tau^\gamma = (k + 1)\gamma \tau^\gamma \leq T^\gamma \).

**Lemma 6.3.** If \( y(t) \in C^2[0, T] \), then

\[
I_0^\gamma y(t_{k+1}) - I_0^\gamma y(t_k) = \frac{\tau^\gamma}{\Gamma(\gamma + 1)} \left\{ b_k^{(\gamma)} y(t_1) + \sum_{j=0}^{k-1} b_{k-j-1}^{(\gamma)} [y(t_{j+2}) - y(t_{j+1})] \right\} + R_{k,\gamma}^{(1)},
\]

(6.8)

where \( |R_{k,\gamma}^{(1)}| \leq C b_k^{(\gamma)} \tau^{1+\gamma} \).

**Proof.** Using Lemma 6.1 and Lemma 6.2, for \( k = 0, 1, \ldots, n - 1 \), we have

\[
I_0^\gamma y(t_{k+1}) - I_0^\gamma y(t_k)
= \frac{1}{\Gamma(\gamma)} \left[ \int_0^{t_{k+1}} \frac{y(\eta)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta - \int_0^{t_k} \frac{y(\eta)}{(t_k - \eta)^{1-\gamma}} d\eta \right]
= \frac{1}{\Gamma(\gamma)} \left[ \int_0^\tau \frac{y(\eta)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta + \int_0^{t_k} \frac{y(\eta + \tau) - y(\eta)}{(t_k - \eta)^{1-\gamma}} d\eta \right]
= \frac{1}{\Gamma(\gamma)} \left[ \int_0^\tau \frac{y(\eta)}{(t_{k+1} - \eta)^{1-\gamma}} d\eta + \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{y(\eta + \tau) - y(\eta)}{(t_k - \eta)^{1-\gamma}} d\eta \right]
= \frac{\tau^\gamma}{\Gamma(\gamma + 1)} \left\{ b_k^{(\gamma)} y(t_1) + \sum_{j=0}^{k-1} b_{k-j-1}^{(\gamma)} [y(t_{j+2}) - y(t_{j+1})] \right\} + R_{k,\gamma}^{(1)},
\]

(6.9)

where \( |R_{k,\gamma}^{(1)}| \leq C b_k^{(\gamma)} \tau^{1+\gamma} \).

Integrating both sides of the Eqn.(6.1) from \( t_k \) to \( t_{k+1} \), we have

\[
u(x_i, t_{k+1}) - u(x_i, t_k) = K [I_0^{\gamma_i} \frac{\partial^2 u(x_i, t_{k+1})}{\partial x^2} - I_0^{\gamma_i} \frac{\partial^2 u(x_i, t_k)}{\partial x^2}]
- \mu^2 [I_0^{\gamma_i} u(x_i, t_{k+1}) - I_0^{\gamma_i} u(x_i, t_k)] + \int_{t_k}^{t_{k+1}} f(x_i, t) dt.
\]

(6.10)
If \( u(x, t) \in C_{x,t}^{4,2}([0, L] \times [0, T]) \), using Lemma 6.3, we have

\[
\begin{align*}
\frac{d}{d t} u(x, t) + \sum_{j=0}^{k-1} b_j^{(1)} u(x, t) + r_1 \sum_{j=0}^{k-1} \delta_x^2 u(x, t) & \quad (\text{6.11}) \\
- r_2 \sum_{j=0}^{k-1} b_j^{(2)} u(x, t) - r_2 \sum_{j=0}^{k-1} \delta_x^2 u(x, t) & \quad (\text{6.12}) \\
\end{align*}
\]

i.e.,

\[
\begin{align*}
u(x, t_{k+1}) = u(x, t_k) + r_1 \sum_{j=0}^{k-1} \delta_x^2 u(x, t_j) + r_1 \sum_{j=0}^{k-1} \left( b_{j+1}^{(1)} - b_j^{(1)} \right) \delta_x^2 u(x, t_{k-j}) \\
- r_2 \left[ f(x, t_{k+1}) + f(x, t_k) \right] + R_{i,k+1}^{1} + R_{i,k+1}^{2},
\end{align*}
\]

where \( r_1 = \frac{K \tau^{(1)}}{\Gamma((1)+1) h^2} \) and \( r_2 = \frac{\mu^2 \tau^{(2)}}{\Gamma((2)+1)} \),

\[
\begin{align*}
|R_{i,k+1}^{1}| & \leq C b_k^{(1)} \tau^{(1)} (\tau + h^2), \\
|R_{i,k+1}^{2}| & \leq C b_k^{(2)} \tau^{(1)} + \tau^{(2)}.
\end{align*}
\]

Thus, we have derived a new implicit numerical method for the initial-boundary value problem of the fractional cable equation:

\[
\begin{align*}
u_{i}^{k+1} = u_{i}^{k} + r_1 \sum_{j=0}^{k-1} \delta_x^2 u_{i}^{k} + r_1 \sum_{j=0}^{k-1} b_{j+1}^{(1)} - b_j^{(1)} \delta_x^2 u_{i}^{k-j} \\
- r_2 \sum_{j=0}^{k-1} b_{j+1}^{(2)} - b_j^{(2)} \delta_x^2 u_{i}^{k-j} \\
+ \frac{\tau}{2} \left[ f(x, t_{k+1}) + f(x, t_k) \right],
\end{align*}
\]

\[
\begin{align*}
i = 1, 2, \ldots, m - 1; \quad k = 0, 1, 2, \ldots, n - 1,
\end{align*}
\]
where \( \delta^2 u_i^k = u_{i+1}^k - 2u_i^k + u_{i-1}^k \). The initial and boundary conditions can be discretised by

\[
\begin{align*}
    u_i^0 &= \phi(ih), \quad i = 0, 1, 2, \ldots, m, \quad (6.15) \\
    u_0^k &= \varphi_1(k\tau), \quad u_m^k = \varphi_2(k\tau), \quad k = 0, 1, 2, \ldots, n. \quad (6.16)
\end{align*}
\]

### 6.3 Stability of the implicit numerical method

For \( u = (u_1, u_2, \ldots, u_{m-1})^T, \ v = (v_1, v_2, \ldots, v_{m-1})^T \), we define

\[
(u, v) = \sum_{j=1}^{m-1} u_j v_j h, \quad \|u\|_2 = \sqrt{(u, u)} = (\sum_{j=1}^{m-1} u_j^2 h^2)^{\frac{1}{2}}. \quad (6.17)
\]

For \( u_0, u_1, \ldots, u_m \), we introduce the following notations:

\[
\Delta_x u_i = u_{i+1} - u_i, \quad \Delta_x u = (\Delta_x u_1, \Delta_x u_2, \ldots, \Delta_x u_{m-1})^T. \quad (6.18)
\]

**Lemma 6.4.** [166] Let \( u = (u_1, u_2, \ldots, u_{m-1})^T, \ v = (v_1, v_2, \ldots, v_{m-1})^T \) and assume that \( u_0 = 0 \) and \( v_m = 0 \), then

\[
(\delta^2 u, v) = -u_1 v_1 h - (\Delta_x u, \Delta_x v). \quad (6.19)
\]

Now we define a new energy norm and prove the following theorem of stability.

**Theorem 6.1.** The implicit numerical method defined by Eqn.(6.14)-(6.16) is unconditionally stable.

**Proof.** We suppose that \( \tilde{u}_i^k \), \( i = 0, 1, 2, \ldots, m, \ (k = 0, 1, 2, \ldots, n) \) is the approximate solution of Eqn.(6.14)-(6.16). The rounding error \( \varepsilon_i^k = \tilde{u}_i^k - u_i^k \) satisfies

\[
\varepsilon_i^{k+1} = \varepsilon_i^k + r_1 \delta^2 \varepsilon_i^{k+1} + r_1 \sum_{j=0}^{k-1} (b_j^{(\gamma_1)} - b_j^{(\gamma_1)}) \delta^2 \varepsilon_i^{k-j} - r_2 \varepsilon_i^{k+1} - r_2 \sum_{j=0}^{k-1} (b_j^{(\gamma_2)} - b_j^{(\gamma_2)}) \varepsilon_i^{k-j}, \quad (6.20)
\]
and \( \varepsilon_0^k = \varepsilon_m^k = 0, \ (k = 0, 1, \ldots, n). \)

Let \( E^k = (\varepsilon_1^k, \varepsilon_2^k, \ldots, \varepsilon_{m-1}^k)^T \). Multiplying Eqn.(6.17) by \( h \varepsilon_i^{k+1} \) and summing for \( i \) from 1 to \( m - 1 \), using Lemma 6.4 we obtain

\[
\|E^{k+1}\|_2^2 = (E^{k+1}, E^k) + r_1 (\delta^2 E^{k+1}, E^{k+1}) \\
+ r_1 \sum_{j=0}^{k-1} (b_j^{(\gamma_1)} - b_j^{(\gamma_1)}) (\delta^2 E^{k-j}, E^{k+1}) \\
- r_2 (E^{k+1}, E^{k+1}) - r_2 \sum_{j=0}^{k-1} (b_j^{(\gamma_2)} - b_j^{(\gamma_2)}) (E^{k-j}, E^{k+1})
\]

\[
= (E^{k+1}, E^k) - r_1 \left[ \|\varepsilon_1^{k+1}\|^2 h + \|\Delta_x E^{k+1}\|_2^2 \right] \\
+ r_1 \sum_{j=0}^{k-1} (b_j^{(\gamma_1)} - b_j^{(\gamma_1)}) \left[ -\varepsilon_1^{k-j} \varepsilon_1^{k+1} h - (\Delta_x E^{k-j}, \Delta_x E^{k+1}) \right] \\
- r_2 (E^{k+1}, E^{k+1}) - r_2 \sum_{j=0}^{k-1} (b_j^{(\gamma_2)} - b_j^{(\gamma_2)}) (E^{k-j}, E^{k+1}). \quad (6.21)
\]

Using Cauchy-Schwarz inequality, we have

\[
\pm \left( \Delta_x E^{k-j}, \Delta_x E^{k+1} \right) \leq \frac{1}{2} \left( \|\Delta_x E^{k-j}\|_2^2 + \|\Delta_x E^{k+1}\|_2^2 \right), \quad (6.22)
\]

\[
\pm \varepsilon_1^{k-j} \varepsilon_1^{k+1} \leq \frac{1}{2} \left( \|\varepsilon_1^{k-j}\|^2 + \|\varepsilon_1^{k+1}\|^2 \right). \quad (6.23)
\]

Thus, we have

\[
\|E^{k+1}\|_2^2 \leq \frac{1}{2} \left( \|E^{k+1}\|_2^2 + \|E^k\|_2^2 \right) - r_1 \|\varepsilon_1^{k+1}\|^2 h - r_1 \|\Delta_x E^{k+1}\|_2^2 \\
+ \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j^{(\gamma_1)} - b_j^{(\gamma_1)}) \|\varepsilon_1^{k+1}\|^2 h + \|\varepsilon_1^{k-j}\|^2 h \\
+ \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j^{(\gamma_1)} - b_j^{(\gamma_1)}) \left[ \|\Delta_x E^{k-j}\|_2^2 + \|\Delta_x E^{k+1}\|_2^2 \right] \\
- r_2 \|E^{k+1}\|_2^2 \\
+ \frac{r_2}{2} \sum_{j=0}^{k-1} (b_j^{(\gamma_2)} - b_j^{(\gamma_2)}) \left[ \|E^{k-j}\|_2^2 + \|E^{k+1}\|_2^2 \right]. \quad (6.24)
\]

Noting \( b_0^\gamma = 1 \), we have

\[
\sum_{j=0}^{k-1} (b_j^{(\gamma)} - b_j^{(\gamma)}) = 1 - b_k^{(\gamma)}, \quad (6.25)
\]
and

\[
\|E^{k+1}\|_2^2 \leq \frac{1}{2}\left[\|E^{k+1}\|_2^2 + \|E^k\|_2^2\right] - \frac{r_1}{2}(1 + b_k^{(\gamma_1)})\|\varepsilon_1^{k+1}\|_2^2 h + \|\Delta_x E^{k+1}\|_2^2 \\
+ \frac{r_1}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma_1)} - b_{j+1}^{(\gamma_1)})\|\varepsilon_1^{k-j}\|_2^2 h + \|\Delta_x E^{k-j}\|_2^2 \\
- \frac{r_2}{2}(1 + b_k^{(\gamma_2)})\|E^{k+1}\|_2^2 + \frac{r_2}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma_2)} - b_{j+1}^{(\gamma_2)})\|E^{k-j}\|_2^2 \\
\leq \frac{1}{2}\left[\|E^{k+1}\|_2^2 + \|E^k\|_2^2\right] - \frac{r_1}{2}\|\varepsilon_1^{k+1}\|_2^2 h + \|\Delta_x E^{k+1}\|_2^2 \\
+ \frac{r_1}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma_1)} - b_{j+1}^{(\gamma_1)})\|\varepsilon_1^{k-j}\|_2^2 h + \|\Delta_x E^{k-j}\|_2^2 \\
- \frac{r_2}{2}\|E^{k+1}\|_2^2 + \frac{r_2}{2}\sum_{j=0}^{k-1}(b_j^{(\gamma_2)} - b_{j+1}^{(\gamma_2)})\|E^{k-j}\|_2^2.
\]

(6.26)

Therefore, we obtain

\[
\|E^{k+1}\|_2^2 + r_1\sum_{j=0}^{k} b_j^{(\gamma_1)}\|\varepsilon_1^{k+1-j}\|_2^2 h + \|\Delta_x E^{k+1-j}\|_2^2 + r_2\sum_{j=0}^{k-1} b_j^{(\gamma_2)}\|E^{k-j}\|_2^2 \\
\leq \|E^k\|_2^2 + r_1\sum_{j=0}^{k-1} b_j^{(\gamma_1)}\|\varepsilon_1^{k-j}\|_2^2 h + \|\Delta_x E^{k-j}\|_2^2 + r_2\sum_{j=0}^{k-1} b_j^{(\gamma_2)}\|E^{k-j}\|_2^2.
\]

(6.27)

By defining the new energy norm

\[
\|E^k\|_E^2 = \|E^k\|_2^2 + r_1\sum_{j=0}^{k-1} b_j^{(\gamma_1)}\|\varepsilon_1^{k-j}\|_2^2 h + \|\Delta_x E^{k-j}\|_2^2 + r_2\sum_{j=0}^{k-1} b_j^{(\gamma_2)}\|E^{k-j}\|_2^2,
\]

(6.28)

we obtain the result

\[
\|E^{k+1}\|_2^2 \leq \|E^{k+1}\|_E^2 \leq \|E^k\|_E^2 \leq \cdots \leq \|E^1\|_E^2 = \|E^0\|_2^2.
\]

Hence, this completes the proof.
6.4 Convergence of the implicit numerical method

In this section, we discuss the convergence of the implicit numerical method.

Let \( u(x_i, t_k) \) \((i = 0, 1, 2, \ldots, m; \ k = 0, 1, 2, \ldots, n)\) be the exact solution of the fractional cable equation (6.1) - (6.3) at mesh point \((x_i, t_k)\). Define \( \eta_i^k = u(x_i, t_k) - u_i^k \), \( i = 0, 1, 2, \ldots, m; \ k = 0, 1, 2, \ldots, n \) and \( Y^k = (\eta_1^k, \eta_2^k, \ldots, \eta_{m-1}^k)^T \).

Lemma 6.5. \cite{166} Let \( \|Y^k\|_\infty = \max_{1 \leq i \leq m-1} |\eta_i^k| \), then

\[
\|Y^k\|_2 \leq L\|Y^k\|_\infty \leq \frac{L^2}{2h^2} \left[ h|\eta_1^k|^2 + \|\Delta_x Y^k\|_2^2 \right].
\]

Now we define a new energy norm and prove the following theorem of convergence.

**Theorem 6.2.** Suppose that \( u(x, t) \in C^{4,2}_{x,t}([0, L] \times [0, T]) \), then the implicit numerical method defined by Eqn.(6.14)-(6.16) is convergent, and there exists a positive constant \( C^* > 0 \), such that

\[
\|Y^{k+1}\|_2 \leq C^*(\tau + h^2), \ k = 0, 1, 2, \ldots, n - 1.
\] (6.29)

**Proof.** From Eqn.(6.12) and Eqn.(6.14), we have

\[
\eta_i^{k+1} = \eta_i^k + r_1 \delta_x^2 \eta_i^{k+1} + r_1 \sum_{j=0}^{k-1} (b_{j+1}^{(\gamma_1)} - b_j^{(\gamma_1)}) \delta_x^2 \eta_i^{k-j} - r_2 \eta_i^{k+1} - r_2 \sum_{j=0}^{k-1} (b_{j+1}^{(\gamma_2)} - b_j^{(\gamma_2)}) \eta_i^{k-j} + R_{i,k+1}^{\gamma_1} + R_{i,k+1}^{\gamma_2},
\] (6.30)

where \( i = 1, 2, \ldots, m - 1; \ k = 0, 1, 2, \ldots, n - 1 \), and

\[
\eta_i^0 = 0, \ i = 0, 1, \ldots, m, \quad (6.31)
\]

\[
\eta_i^k = \eta_i^{k} = 0, \ k = 0, 1, \ldots, n. \quad (6.32)
\]
Multiplying Eqn. (6.30) by $h \eta_i^{k+1}$ and summing up for $i$ from 1 to $m - 1$, we obtain

\[
\|Y^{k+1}\|_2^2 = (Y^{k+1}, Y^k) + r_1 (\sigma_2 Y^{k+1}, Y^{k+1}) + r_1 \sum_{j=0}^{k-1} (b_j^{(\gamma_1)} - b_j^{(\gamma_1)}) (\delta_2 Y^{k-j}, Y^{k+1})
\]

\[-r_2 (Y^{k+1}, Y^{k+1}) - r_2 \sum_{j=0}^{k-1} (b_j^{(\gamma_2)} - b_j^{(\gamma_2)}) (Y^{k-j}, Y^{k+1})
\]

\[+(R_{k+1}^{\gamma_1}, Y^{k+1}) + (R_{k+1}^{\gamma_2}, Y^{k+1}) \leq \frac{1}{2} \left[ \|Y^{k+1}\|_2^2 + \|Y^k\|_2^2 \right] - \frac{r_1}{2} (1 + b_k^{(\gamma_1)}) \left[ \eta_i^{k+1} h + \|\Delta_x Y^{k+1}\|_2^2 \right]
\]

\[+ \frac{r_1}{2} \sum_{j=0}^{k-1} (b_j^{(\gamma_1)} - b_{j+1}^{(\gamma_1)}) \left( \eta_i^{k-j} h + \|\Delta_x Y^{k-j}\|_2^2 \right)
\]

\[-\frac{r_2}{2} (1 + b_k^{(\gamma_2)}) \|Y^{k+1}\|_2^2 + \frac{r_2}{2} \sum_{j=0}^{k-1} (b_j^{(\gamma_2)} - b_{j+1}^{(\gamma_2)}) \|Y^{k-j}\|_2^2
\]

\[+(R_{k+1}^{\gamma_1}, Y^{k+1}) + (R_{k+1}^{\gamma_2}, Y^{k+1}). \quad (6.33)
\]

Define the new energy norm

\[
\|Y^k\|_E^2 = \|Y^k\|_2^2 + r_1 \sum_{j=0}^{k-1} b_j^{(\gamma_1)} \left( \eta_i^{k-j} h + \|\Delta_x Y^{k-j}\|_2^2 \right) + r_2 \sum_{j=0}^{k-1} b_j^{(\gamma_2)} \|Y^{k-j}\|_2^2.
\]

(6.34)

Using $|uv| \leq \sigma u^2 + \frac{1}{4\sigma} v^2$, $\sigma > 0$, we have

\[(R_{k+1}^{\gamma_1}, Y^{k+1}) \leq \frac{r_1 h^2 b_k^{(\gamma_1)}}{L^2} \|Y^{k+1}\|_2^2 + \frac{L^2}{4r_1 h^2 b_k^{(\gamma_1)}} \|R_{k+1}^{\gamma_1}\|_2^2, \quad (6.35)
\]

\[(R_{k+1}^{\gamma_2}, Y^{k+1}) \leq \frac{r_2 b_k^{(\gamma_2)}}{2} \|Y^{k+1}\|_2^2 + \frac{1}{2r_2 b_k^{(\gamma_2)}} \|R_{k+1}^{\gamma_2}\|_2^2, \quad (6.36)
\]

and

\[\|R_{k+1}^{\gamma_1}\|_2 = \sqrt{\sum_{i=1}^{m-1} |R_{i,k+1}^{\gamma_1}|^2} \leq C b_k^{(\gamma_1)} \tau^{\gamma_1} (\tau + h^2), \quad (6.37)
\]

\[\|R_{k+1}^{\gamma_2}\|_2 = \sqrt{\sum_{i=1}^{m-1} |R_{i,k+1}^{\gamma_2}|^2} \leq C b_k^{(\gamma_2)} \tau^{1+\gamma_2}. \quad (6.38)
\]
Applying Lemma 6.5, we have

$$\frac{r_1 h^2 b_k^{(\gamma_1)}}{L^2} \|Y^{k+1}\|^2 \leq \frac{b_k^{(\gamma_1)} r_1}{2} \left[ \eta_1^{k+1} h + \Delta_x Y^{k+1} \right].$$

(6.39)

Therefore, we obtain

$$\|Y^{k+1}\|^2 \leq \|Y^{k}\|^2 + r_1 \sum_{j=0}^{k} b_j^{(\gamma_1)} \left[ \eta_1^{k+1-j} h + \Delta_x Y^{k+1-j} \right] + r_2 \sum_{j=0}^{k} b_j^{(\gamma_2)} \|Y^{k+1-j}\|^2$$

$$\leq \|Y^{k}\|^2 + r_1 \sum_{j=0}^{k} b_j^{(\gamma_1)} \left[ \eta_1^{k+1-j} h + \Delta_x Y^{k+1-j} \right] + r_2 \sum_{j=0}^{k} b_j^{(\gamma_2)} \|Y^{k+1-j}\|^2$$

$$\leq \|Y^{k}\|^2 - \frac{r_1}{2} b_k^{(\gamma_1)} \left[ \eta_1^{k+1} h + \Delta_x Y^{k+1} \right] - \frac{r_2}{2} b_k^{(\gamma_2)} \|Y^{k+1}\|^2$$

$$\leq \|Y^{k}\|^2 + \frac{r_1}{2} b_k^{(\gamma_1)} \left[ \eta_1^{k+1} h + \Delta_x Y^{k+1} \right] - \frac{r_2}{2} b_k^{(\gamma_2)} \|Y^{k+1}\|^2$$

$$\leq \|Y^{0}\|^2 + C \sum_{j=0}^{k} b_j^{(\gamma_1)} \tau_1 (\tau + h^2) + C \sum_{j=0}^{k} b_j^{(\gamma_2)} \tau_2 \tau$$

$$\leq \|Y^{0}\|^2 + C \left[ \tau_1 (\tau + h^2) \right]^2,$$

(6.40)

i.e., \(\|Y^{k+1}\| \leq \|Y^{k+1}\|_E \leq C^* (\tau + h^2).\)

Hence, this completes the proof of convergence.

### 6.5 An improved implicit numerical method

In this section, we present an improved implicit numerical method for the fractional cable equation.
Lemma 6.6. If the function $y(t)$ is sufficiently smooth, then

$$y(\eta) = \frac{(t_{j+1} - \eta)y(t_j) + (\eta - t_j)y(t_{j+1})}{\tau} + O(\tau^2).$$

(6.41)

Thus, we have

$$I_0^\gamma y(t_k) = \frac{1}{\Gamma(\gamma)} \sum_{j=0}^{k-1} \int_{t_j}^{t_{j+1}} \frac{y(\eta)}{(t_k - \eta)^{1-\gamma}} d\eta,$$

$$= \frac{\tau^\gamma}{\Gamma(\gamma + 1)} \sum_{j=0}^{k-1} \left[ a^\gamma_j y(t_{k-j-1}) + c^\gamma_j y(t_{k-j}) \right] + \tilde{R}^\gamma_k$$

(6.42)

where

$$a^\gamma_j = (j + 1)^\gamma - \frac{1}{\gamma + 1} \left[ (j + 1)^{\gamma+1} - j^{\gamma+1} \right],$$

(6.43)

$$c^\gamma_j = \frac{1}{\gamma + 1} \left[ (j + 1)^{\gamma+1} - j^{\gamma+1} \right] - j^\gamma,$$

(6.44)

$$|\tilde{R}^\gamma_k| = O(\tau^2).$$

(6.45)

From Eqn.(6.7) and Eqn.(6.42), we have

$$u(x_i, t_{k+1}) - u(x_i, t_k) = K \left[ I_0^{\gamma_1} \frac{\partial^2 u(x_i, t_{k+1})}{\partial x^2} - I_0^{\gamma_1} \frac{\partial^2 u(x_i, t_k)}{\partial x^2} \right]$$

$$- \mu^2 \left[ I_0^{\gamma_2} u(x_i, t_{k+1}) - I_0^{\gamma_2} u(x_i, t_k) \right] + \int_{t_k}^{t_{k+1}} f(x_i, t) dt$$

$$= r_1 \sum_{j=0}^{k} \left[ a^{\gamma_2}_j \delta^2_x u(x_i, t_{k-j}) + c^{\gamma_2}_j \delta^2_x u(x_i, t_{k-j+1}) \right]$$

$$- r_1 \sum_{j=0}^{k-1} \left[ a^{\gamma_1}_j \delta^2_x u(x_i, t_{k-j-1}) + c^{\gamma_1}_j \delta^2_x u(x_i, t_{k-j}) \right]$$

$$- r_2 \sum_{j=0}^{k} \left[ a^{\gamma_2}_j u(x_i, t_{k-j}) + c^{\gamma_2}_j u(x_i, t_{k-j+1}) \right]$$

$$+ r_2 \sum_{j=0}^{k-1} \left[ a^{\gamma_2}_j u(x_i, t_{k-j-1}) + c^{\gamma_2}_j u(x_i, t_{k-j}) \right]$$

$$+ \frac{\tau}{2} \left[ f(x_i, t_{k+1}) + f(x_i, t_k) \right] + \tilde{R}_{i,k+1},$$

(6.46)
6.6 Numerical results

Table 6.1: The error $\|Y^k\|_2$ between the exact solution and the numerical solution (INM) and the effect of the grid size reduction at time $T = 1.0 \ (\gamma_1 = \gamma_2 = 0.5)$

<table>
<thead>
<tr>
<th>$h$</th>
<th>$\tau$</th>
<th>$L_2$ norm error of INM</th>
<th>Error rate of INM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>0.04</td>
<td>4.3047E-3</td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>0.01</td>
<td>1.4197E-3</td>
<td>3.032</td>
</tr>
<tr>
<td>0.05</td>
<td>0.0025</td>
<td>3.9777E-4</td>
<td>3.569 $\approx$ 4</td>
</tr>
<tr>
<td>0.025</td>
<td>0.000625</td>
<td>1.0481E-4</td>
<td>3.795 $\approx$ 4</td>
</tr>
</tbody>
</table>

Table 6.2: The error $\|Y^k\|_2$ between the exact solution and the numerical solution (IINM) and the effect of the grid size reduction at time $T = 1.0 \ (\gamma_1 = \gamma_2 = 0.5)$

<table>
<thead>
<tr>
<th>$h$</th>
<th>$\tau$</th>
<th>$L_2$ norm error of IINM</th>
<th>Error rate of IINM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.04</td>
<td>0.04</td>
<td>7.4129E-4</td>
<td></td>
</tr>
<tr>
<td>0.02</td>
<td>0.02</td>
<td>1.8525E-4</td>
<td>4.002 $\approx$ 4</td>
</tr>
<tr>
<td>0.01</td>
<td>0.01</td>
<td>4.6307E-5</td>
<td>3.995 $\approx$ 4</td>
</tr>
<tr>
<td>0.005</td>
<td>0.005</td>
<td>1.1577E-5</td>
<td>4.005 $\approx$ 4</td>
</tr>
<tr>
<td>0.0025</td>
<td>0.0025</td>
<td>2.8941E-6</td>
<td>4.000 $\approx$ 4</td>
</tr>
</tbody>
</table>

where $R_{i,k+1} = O(\tau^2 + h^2)$. Thus, we obtain the improved implicit numerical method:

\[
\begin{align*}
&u_i^{k+1} - u_i^k \\
= r_1 \left\{ a_{0}^{\gamma_1} \delta_x^2 u_i^k + c_{0}^{\gamma_1} \delta_x^2 u_i^{k+1} + \sum_{j=0}^{k-1} \left[ (a_{j+1}^{\gamma_1} - a_j^{\gamma_1}) \delta_x^2 u_i^{k-j-1} + (c_{j+1}^{\gamma_1} - c_j^{\gamma_1}) \delta_x^2 u_i^{k-j} \right] \right\} \\
- r_2 \left\{ a_0^{\gamma_2} u_i^k + c_0^{\gamma_2} u_i^{k+1} + \sum_{j=0}^{k-1} \left[ (a_{j+1}^{\gamma_2} - a_j^{\gamma_2}) u_i^{k-j-1} + (c_{j+1}^{\gamma_2} - c_j^{\gamma_2}) u_i^{k-j} \right] \right\} \\
+ \frac{\tau}{2} \left( f_i^{k+1} + f_i^k \right). 
\end{align*}
\]

6.6 Numerical results

In order to demonstrate the effectiveness of both implicit numerical methods, some examples are now presented.

**Example 6.1.** Consider the following initial and boundary problem of the fractional cable equation

\[
\frac{\partial u(x, t)}{\partial t} = 0 D_{t}^{1-\gamma_1} \frac{\partial^2 u(x, t)}{\partial x^2} - 0 D_{t}^{1-\gamma_2} u(x, t) + f(x, t),
\]

\[
u(x, 0) = 0, \quad 0 \leq x \leq 1,
\]

\[
u(0, t) = 0, \quad u(1, t) = 0, \quad 0 \leq t \leq T,
\]

where \( f(x, t) = 2(t + \frac{\pi^2}{\Gamma(2+\gamma_1)} t^{1+\gamma_1} + \frac{t^{1+\gamma_2}}{\Gamma(2+\gamma_2)}) \sin \pi x. \)
The exact solution of Eqn. (6.48)-(6.50) is \( u(x, t) = t^2 \sin \pi x \), which can be obtained by evaluating the fractional derivative formula [114].

In this example, we define the following \( L^2 \) norm numerical error:

\[
\|Y^k\|_2 = \left[ \sum_{i=0}^{m} |u(x_i, t_k) - u^k_i|^2 h \right]^{1/2}.
\] (6.51)

The numerical errors with \( \gamma_1 = \gamma_2 = 0.5 \) at \( T = 1.0 \) using the implicit numerical method (INM) with convergence order \( O(\tau + h^2) \) and the improved implicit numerical method (IINM) with convergence order \( O(\tau^2 + h^2) \) are shown in Tables 6.1 and 6.2, respectively. It can be seen that both numerical methods are in excellent agreement with the exact solution.

From Tables 6.1 and 6.2, it can be seen that

\[
\text{Error Rate of INM} = \frac{\text{error}_1}{\text{error}_2} \approx \frac{\tau_1}{\tau_2} = \left( \frac{h_1}{h_2} \right)^2 = 4
\]

and

\[
\text{Error Rate of IINM} = \frac{\text{error}_1}{\text{error}_2} \approx \left( \frac{\tau_1}{\tau_2} \right)^2 = \left( \frac{h_1}{h_2} \right)^2 = 2^2.
\]

Thus, we obtain that the order of convergence of the numerical method INM are \((\log_4 4 = 1)\) for \( \tau \) and \((\log_2 4 = 2)\) for \( h \), i.e., the order of convergence of INM is \( O(\tau + h^2) \); and the order of convergence of the numerical method IINM are \((\log_2 4 = 2)\) for \( \tau \) and \((\log_2 4 = 2)\) for \( h \), i.e., the order of convergence of IINM is \( O(\tau^2 + h^2) \). These results are in good agreement with our theoretical analysis.

Example 6.2. Consider the following initial and boundary problem of the fractional cable equation

\[
\begin{align*}
\frac{\partial u(x, t)}{\partial t} &= 0D_t^{1-\gamma_1} \left( K \frac{\partial^2 u(x, t)}{\partial x^2} \right) - \mu^2_0 D_t^{1-\gamma_2} u(x, t), \\
u(x, 0) &= c_0 \delta(x) \\
u(0, t) &= u(L, t) = 0, \quad 0 \leq t \leq T.
\end{align*}
\] (6.52)
Figure 6.1: Plot of $u(x, t)$ versus $x$ for $\gamma_1 = \gamma_2 = 0.5$ (solid line) and $\gamma_1 = \gamma_2 = 1.0$ (dotted line) at different times $T = 0.1, 0.5$.

In this example, we let $K = 1$, $\mu^2 = 0.5$, $L = 10$, $c_0 = 10$, and $\delta(x)$ be the Dirac delta function. First, we consider the case of $\gamma_1 = \gamma_2$. From Figure 6.1, we see that the solution profile $u(x, t)$ is characterised by a sharp peak and a heavy tail. Furthermore, in this fractional cable model, the peak height decreases more rapidly as $\gamma_1 (= \gamma_2)$ is decreased at the early time $T = 0.1$, but this trend reverses for the later time $T = 0.5$. These results are consistent with those found in Henry et al. [54], and they point out that these results are important for addressing the electrotonic significance of decreasing spine densities.

However, Henry et al. [54] did not consider the case of $\gamma_1 \neq \gamma_2$. We remark that using our numerical methods enables the case $\gamma_1 \neq \gamma_2$ to be studied, which can be used to investigate other interesting properties of the fractional cable model. For example, we can investigate the different impacts of $\gamma_1$ and $\gamma_2$ on the anomalous behaviour. Figure 6.2 shows the changes in the solution profiles when $\gamma_1$ is fixed at 0.1 and $\gamma_2$ is varied from 0.2 to 1.0 at time $T = 0.1$. Figure 6.3 displays the changes in the solution profiles when $\gamma_2$ is fixed at 0.8 and $\gamma_1$ is varied from 0.2 to 1.0 at time $T = 0.1$. From the representative results, we see there is a crossover between more and less anomalous behaviour.

Calibration and validation of the fractional cable models should provide new insight into the functional implications of altered neuronal spine densities, a hallmark of normal ageing and many neurodegenerative disorders [64, 32, 113].
Figure 6.2: Plot of $u(x, t)$ versus $x$ for fixed $\gamma_1 = 0.1$ and different $\gamma_2 = 0.2, 0.4, 0.6, 0.8, 1.0$ at time $T = 0.1$. $\gamma_2$ increases in the direction of the arrow.

Figure 6.3: Plot of $u(x, t)$ versus $x$ for fixed $\gamma_2 = 0.8$ and different $\gamma_1 = 0.2, 0.4, 0.6, 0.8, 1.0$ at time $T = 0.1$. $\gamma_1$ increases in the direction of the arrow.
6.7 Conclusions

The fractional cable equation has been introduced to model electrotonic properties of spiny neuronal dendrites by many researchers. In this paper, we proposed two new implicit numerical methods to solve the fractional cable equation, with convergence order $O(\tau + h^2)$ and $O(\tau^2 + h^2)$, respectively. We proved the stability and convergence of the implicit numerical method with convergence order $O(\tau + h^2)$ using the energy method by introducing two new energy forms. We also presented two numerical examples to demonstrate the effectiveness of both implicit numerical methods, and to illustrate the changes in solution profiles that arise when the exponent $\gamma_1$ and $\gamma_2$ is varied from integer order to fractional order. Furthermore, the numerical techniques presented have enabled the case $\gamma_1 \neq \gamma_2$ to be simulated, which can be used to investigate the different impacts of $\gamma_1$ and $\gamma_2$ on the anomalous behaviour. From the representative results we see there is a crossover between more and less anomalous behaviour. We believe that this finding is another new contribution to the literature. These numerical techniques can also be applied to solve other types of the anomalous subdiffusion problems with fractional order temporal operators.
Novel numerical methods for solving the time-space fractional diffusion equation in 2D

7.1 Introduction

During the past three decades, the subject of fractional calculus (that is, calculus of integrals and derivatives of arbitrary order) has gained considerable popularity and importance, mainly due to its demonstrated applications in numerous diverse and widespread fields in science, engineering and finance. For example, fractional calculus has been successfully applied to problems in system biology [159], physics [11, 108, 110, 128, 160], chemistry and biochemistry [156], hydrology [13, 14, 78], medicine [54, 99, 53], and finance [51, 120, 132, 148, 107].

A number of numerical methods for solving the time, or space, or time-space fractional partial differential equations have now been proposed [168, 167, 92, 24, 87, 75, 150, 152, 149, 151, 88, 20, 166, 21, 154, 90, 91, 163, 22]. The dominant numerical methods for solving fractional partial differential equations are based on the finite difference method. However, because the fractional derivative is a non-local operator, it is challenging to harness the long history involving classical numerical techniques, such as, finite element method, finite volume method, or
Chapter 7. Novel numerical methods for solving TSFDE-2D

the new meshfree method, to solve fractional partial differential equations. This paper makes an important contribution to the literature by demonstrating how the matrix transform method (MTM) may be used for this purpose.

Two novel numerical methods are proposed for solving the two-dimensional time-space fractional diffusion equation. We suggest a way that classical numerical methods can be used for the spatial discretisation of the fractional derivative. To elucidate these ideas, we consider the following two-dimensional time-space fractional diffusion equation (TSFDE-2D) with homogeneous Dirichlet boundary conditions, and given initial condition:

\[
\begin{align*}
\mathcal{D}_t^\gamma u(x,y,t) &= -K_\alpha (-\Delta)^{\alpha/2} u(x,y,t), \quad 0 < \gamma < 1, \quad 1 < \alpha \leq 2, \quad (7.1) \\
u(0,y,t) &= u(a,y,t) = 0, \quad 0 \leq y \leq b, \quad 0 < t \leq T, \quad (7.2) \\
u(x,0,t) &= u(x,b,t) = 0, \quad 0 \leq x \leq a, \quad 0 < t \leq T \quad (7.3) \\
u(x,y,0) &= u_0(x,y), \quad (7.4)
\end{align*}
\]

where the Laplacian operator is defined as 

\[-\Delta = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}; \quad u\] is, for example, a solute concentration; and \(K_\alpha\) represents the diffusion coefficient.

\(\mathcal{D}_t^\gamma\) is the Caputo fractional derivative of order \(\gamma\) \((0 < \gamma < 1)\) with respect to \(t\) and with the starting point at \(t = 0\) is defined as \([116]\):

\[
\mathcal{D}_t^\gamma u(x,y,t) = \frac{1}{1-\gamma} \int_0^t \frac{u_t(x,y,\tau)}{(t-\tau)^\alpha} d\tau. \quad (7.5)
\]

The symmetric space fractional derivative \(-(-\Delta)^{\alpha/2}\) of order \(\alpha\) \((1 < \alpha \leq 2)\) is a fractional Laplacian operator defined through the eigenfunction expansion on a finite domain (see Definition 7.1 or [61]).

We remark that there is another definition for the fractional Laplacian operator given in the literature, utilising the Fourier transform on an infinite domain [129], with a natural extension to finite domains when the function is subject to homogeneous Dirichlet boundary conditions. It is essential to choose an appropriate numerical method of approximation according to which definition is intended. Yang et al. [150] show that using this alternative definition, the one-dimensional fractional Laplacian operator \(-(-\Delta)^{\alpha/2}\) is equivalent to the Riesz fractional derivative \(\frac{\partial^\alpha}{\partial |x|^\alpha}\) under homogeneous Dirichlet boundary conditions, and hence can be
approximated by the standard/shifted Grünwald method and the L1/L2 approximation.

To solve the TSFDE-2D (7.1)-(7.4), we first introduce a mesh and discretise in space using either the finite difference or finite element methods to obtain an approximate matrix representation $A$ of the Laplacian $(-\Delta)$. We then use the matrix transform method (MTM) proposed by Ilić et al. [61] to transform the TSFDE-2D into a time fractional differential system involving matrix $A$ raised to the fractional index $\alpha/2$ as

$$tD^\gamma u = -K_\alpha A^{\alpha/2}u.$$

We then propose two numerical schemes to solve this equation using either the finite difference method or Laplace transform method, which necessitates the computation of a matrix function vector product $f(A)b$ at each time step. We show how this product can be approximated and give algorithms for each scheme that can easily be adapted for MATLAB.

The rest of this paper is organised as follows. In Section 7.2, we use the MTM to discretise the fractional Laplacian in space. The TSFDE-2D (7.1)-(7.4) is then transformed into a time fractional differential system. Using either the finite difference method or the Laplace transform method to approximate the Caputo time fractional derivative, the solution of the TSFDE-2D is written in terms of a matrix function vector product $f(A)b$ at each time step, where $b$ is a suitably defined vector. In Section 7.3, the adaptively preconditioned Lanczos method and the incomplete Cholesky preconditioned M-Lanczos method are used to approximate the product $f(A)b$. The error bounds for the two newly proposed numerical schemes are also derived in Section 7.3. The analytical solution of the TSFDE-2D is derived in Section 7.4. Finally, numerical experiments are carried out in Section 7.5 to assess the computational performance and accuracy of our new schemes, and some conclusions are drawn in Section 7.6.

### 7.2 Numerical solutions for the TSFDE-2D

In this section, we present two numerical schemes to simulate the solution behaviour of the TSFDE-2D (7.1)–(7.3). In Section 7.2.1, the matrix transform method (MTM) is introduced to discretise the fractional Laplacian. In Section 7.2.2 a finite difference method (FDM) is used to discretise the Caputo time fractional derivative. Section 7.2.3 shows how the first numerical
scheme is derived, by combining the FDM and MTM to transfer the TSFDE-2D (7.1) into a
discrete system describing the evolution of \( u(x, y, t) \) in space and time. Finally, in Section
7.2.4 the second numerical scheme, employing the Laplace transform method (LTM) together
with the MTM is presented.

7.2.1 Matrix transform method in space

We utilise the matrix transform method (MTM) proposed by Ilić et al. [60, 61] to discretise in
space. In this paper the symbol \((-\Delta)^{\alpha/2}\) has the usual meaning as a function of \((-\Delta)\), which is
defined in terms of its spectral decomposition. For boundary value problems on finite domains,
discrete eigenfunction expansions are used, where the following definition is adopted.

**Definition 7.1.** [61] Suppose the two-dimensional Laplacian \((-\Delta)\) has a complete set of or-
thonormal eigenfunctions \(\varphi_{n,m}\) corresponding to eigenvalues \(\lambda_{n,m}\) in a rectangular region
\(D = \{(x, y)|0 \leq x \leq a, 0 \leq y \leq b\}\), i.e., \((-\Delta)\varphi_{n,m} = \lambda_{n,m}\varphi_{n,m}; \quad \mathcal{B}(\varphi) = 0 \text{ on } \partial D\), where
\(\mathcal{B}(\varphi)\) is the homogeneous Dirichlet boundary condition. Let

\[
\mathcal{F}_\eta = \left\{ f = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_{n,m} \varphi_{n,m}, \quad c_{n,m} = \langle f, \varphi_{n,m} \rangle, \quad \sum_{n=1}^{\infty} |c_{n,m}|^2 |\lambda_{n,m}|^{\eta/2} < \infty, \quad \eta = \max(\alpha, 0) \right\},
\]

then for any \(f \in \mathcal{F}_\eta\), the two-dimensional fractional Laplacian \((-\Delta)^{\alpha/2}\) is defined by

\[
(-\Delta)^{\alpha/2} f = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_{n,m} (\lambda_{n,m})^{\alpha/2} \varphi_{n,m},
\]

where \(\lambda_{n,m} = \frac{n^2 \pi^2}{a^2} + \frac{m^2 \pi^2}{b^2}\), and \(\varphi_{n,m} = \sin \frac{n\pi x}{a} \sin \frac{m\pi y}{b}\) are the eigenvalues and correspond-
ing eigenfunctions of the two-dimensional Laplacian \((-\Delta)\) for \(n, m = 1, 2, \ldots\).

One notes that the fractional Laplacian \((-\Delta)^{\alpha/2}\) is a non-local operator and any approximation
of it will result in a large dense matrix. One of the attractive advantages of the MTM is the
fact that the sparse approximation of \((-\Delta)\) can be harnessed directly in the numerical solution
technique, which we now explain.

By introducing a mesh and denoting the value of \(u(x, y, t)\) at the \(i\)th node by \(u_i(t)\), and the
vector of such values by \(\mathbf{u}(t)\), the MTM for solving the TSFDE-2D (7.1) proceeds by first
considering the non-fractional equation

\[ \frac{du}{dt} = -Au \]  \hspace{1cm} (7.6)

where \( A \) is the approximate matrix representation of the standard Laplacian \((-\Delta)\) under homogeneous Dirichlet boundary conditions, obtained by using either finite difference or finite element methods. Clearly, \((-\Delta)\) is an unbounded operator, whereas \( A \) is a bounded matrix operator and therefore it is not possible to conclude that \( A \) is a good representation of \((-\Delta)\). However, the resolvents of each operator are bounded and this motivates the thinking that \( A \) is a good approximate representation of \((-\Delta)\). Further discussion on this observation can be found in Simpson et al. [139]. Then under MTM, the fractional Laplacian operator is approximated as

\[ -(-\Delta)^{\alpha/2}u \approx -A^{\alpha/2}u. \]  \hspace{1cm} (7.7)

In summary, the MTM transforms the TSFDE-2D (7.1)-(7.4) into the following time fractional differential system

\[ \gamma D^\alpha_t u = -K_\alpha A^{\alpha/2}u, \quad u(0) = u^0. \]  \hspace{1cm} (7.8)

This method enables the standard finite difference or finite element methods to be utilised for the spatial discretisation of the Laplacian operator, which we now describe in subsections 7.2.1.1 and 7.2.1.2, respectively.

### 7.2.1.1 Finite difference method in space

The standard five-point finite difference stencil with equal grid spacing in both \( x \) and \( y \) directions, i.e., \( h = \frac{a}{M} = \frac{b}{N} \), will result in the block tridiagonal approximate matrix representation
of the Laplacian, namely

$$A = \frac{1}{h^2} \begin{bmatrix} B & -I \\ -I & B & -I \\ & \ddots & \ddots & \ddots \\ & -I & B & -I \\ -I & B \end{bmatrix} \in \mathbb{R}^{(M-1)(N-1)\times(M-1)(N-1)} \quad (7.9)$$

with

$$B = \begin{bmatrix} 4 & -1 \\ -1 & 4 & -1 \\ & -1 & 4 & -1 \\ & & \ddots & \ddots & -1 \\ & & & -1 & 4 \end{bmatrix} \in \mathbb{R}^{(M-1)\times(M-1)} \quad (7.10)$$

### 7.2.1.2 Finite element method in space

In the case of the finite element method, we begin with the following non-fractional governing equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \equiv -(-\Delta)u \text{ in } \Omega, \quad (7.11)$$

for a two-dimensional domain $\Omega = [0,a] \times [0,b]$. The boundary conditions are

$$u = 0, \text{ on } \partial\Omega. \quad (7.12)$$

Multiplying (7.11) by a test function $v$ and integrating over the computational domain $\Omega$ gives

$$\int_{\Omega} \frac{\partial u}{\partial t} v \, d\Omega = -\int_{\Omega} (-\Delta)u \, v \, d\Omega. \quad (7.13)$$

In order to develop the weak form of (7.13), integration by parts is applied to the right hand side to reduce the order of differentiation within the integral. Requiring that the test function $v$
vanishes on $\partial \Omega$, we obtain the weak form
\[
\int_{\Omega} \frac{\partial u}{\partial t} v \, d\Omega = - \int_{\Omega} \nabla u \cdot \nabla v \, d\Omega. \tag{7.14}
\]

Discretisation of the domain in (7.14) is performed using three-node triangular elements, which are also known as the linear triangular elements [68, 85].

Expanding $u(x, y, t)$ in terms of the shape functions $\{\phi_i(x, y)\}_{i=1}^{N}$, we obtain
\[
u(x, y, t) = \sum_{i=1}^{N} u_i(t) \phi_i(x, y), \tag{7.15}
\]
where $N$ is the number of nodes in the mesh. We note from (7.15) that the shape functions are used to interpolate the spatial variation, while the temporal variation is related with the nodal variables.

We take $v = \phi_j$, $j = 1, \ldots, N$ in (7.14), and obtain the discrete formulation
\[
\int_{\Omega} \sum_{i=1}^{N} \frac{d u_i}{d t} \phi_i \phi_j \, d\Omega = - \int_{\Omega} \sum_{i=1}^{N} u_i \nabla \phi_i \cdot \nabla \phi_j \, d\Omega, \quad j = 1, \ldots, N \tag{7.16}
\]
or, upon interchanging summation and integration,
\[
\sum_{i=1}^{N} \frac{d u_i}{d t} \int_{\Omega} \phi_i \phi_j \, d\Omega = - \sum_{i=1}^{N} u_i \int_{\Omega} \nabla \phi_i \cdot \nabla \phi_j \, d\Omega, \quad j = 1, \ldots, N. \tag{7.17}
\]

Introducing the mass matrix $(M)_{ij} = \int_{\Omega} \phi_i \phi_j \, d\Omega$ and the stiffness matrix $(K)_{ij} = \int_{\Omega} \nabla \phi_i \cdot \nabla \phi_j \, d\Omega$, (7.17) can be written
\[
M \frac{d u}{d t} = -Ku, \tag{7.18}
\]
i.e.,
\[
\frac{d u}{d t} = -M^{-1}Ku. \tag{7.19}
\]

Thus, we have derived that the approximate matrix representation of the standard Laplacian for
the finite element method is

\[ A = M^{-1}K. \] (7.20)

Interestingly, although both \( M \) and \( K \) are symmetric positive definite and sparse, not only is \( A \) non-symmetric, it is also dense. Nevertheless, \( A \) is shown in the following proposition to be similar to the symmetric positive matrix \( \tilde{A} = M^{-\frac{1}{2}}KM^{-\frac{1}{2}} \) and therefore its eigenvalues are positive and real, and hence \( A \) itself is positive definite.

**Proposition 7.1.** The matrix \( A = M^{-1}K \) is similar to the symmetric positive matrix \( \tilde{A} = M^{-\frac{1}{2}}KM^{-\frac{1}{2}} \) and is positive definite.

**Proof.** First note that since \( M \in SPD \), \( M = M^{1/2}M^{1/2} \), furthermore \( M^{-1/2}M^{1/2} = I \). The characteristic polynomial of \( A \) is

\[
p_{A}(\lambda) = \det(\lambda I - M^{-1}K)
= \det(\lambda M^{-\frac{1}{2}}M^{\frac{1}{2}} - M^{-\frac{1}{2}}KM^{-\frac{1}{2}}M^{\frac{1}{2}})
= \det(\lambda M^{-\frac{1}{2}}(\lambda I - \tilde{A})M^{\frac{1}{2}})
= \det(\lambda I - \tilde{A}) = p_{\tilde{A}}(\lambda).
\]

Thus the matrix \( A \) and \( \tilde{A} \) have the same real eigenvalues. We now show the eigenvalues are positive.

Consider \( \forall x \neq 0, x^T\tilde{A}x = x^TM^{-\frac{1}{2}}KM^{-\frac{1}{2}}x = y^TKy > 0 \) since \( K \in SPD \). Note \( y = M^{-\frac{1}{2}}x \neq 0 \) since \( x \neq 0 \) and \( M \in SPD \). □

### 7.2.2 Finite difference method in time

We now discretise (7.8) in time using the following scheme. Let \( t_n := n\tau, \ n = 0, 1, 2, \ldots, \) where \( \tau \) is the time step. We adopt the finite difference method (FDM) to discretise the Caputo time fractional derivative as [76]:

\[
\tau D_{\tau}^\gamma u^n = \frac{1}{\mu_0} \sum_{j=0}^{n-1} b_j [u^{n-j} - u^{n-1-j}] + O(\tau^{2-\gamma}),
\] (7.21)
where

\[ \mu_0 = \tau^\gamma \Gamma(2 - \gamma), \tag{7.22} \]

\[ b_j = (j + 1)^{1-\gamma} - j^{1-\gamma}, \quad j = 0, 1, 2, \ldots, n - 1. \tag{7.23} \]

One difficulty with this approach, and indeed in solving time fractional differential equations in general, is that the fractional derivatives are non-local operators. This non-local property means that the next state of the system not only depends on its current state, but also on the historical states starting from the initial time. Hence, applying the scheme (7.21) requires the storage and processing of all previous time steps.

In this work, we assume that the additional memory and computational cost is acceptable. However, we note that some authors have explored techniques for reducing this cost. The simplest approach is to disregard the tail of the integral and to integrate only over a fixed period of recent history. This is commonly referred to as the ‘short-memory’ principle, and is described by Podlubny [116].

### 7.2.3 Finite difference method with matrix transform method

Combining the approximation for the Caputo time fractional derivative (7.21) with the approximation of the fractional Laplacian (7.7), we obtain the following numerical approximation of the TSFDE-2D (7.1):

\[ \mu_0 \sum_{j=0}^{n-1} b_j [u^{n-j} - u^{n-1-j}] = -K_\alpha A^{\alpha/2} u^n. \tag{7.24} \]

After some further manipulations, (7.24) reads

\[ u^n = \left[ I + \mu_0 K_\alpha A^{\alpha/2} \right]^{-1} \left[ \sum_{j=0}^{n-2} (b_j - b_{j+1}) u^{n-1-j} + b_{n-1} u^0 \right]. \tag{7.25} \]

Defining the scalar function \( f_1(\xi) = \left[ 1 + \mu_0 K_\alpha \xi^{\alpha/2} \right]^{-1} \), we obtain the first numerical scheme
for approximating the TSFDE-2D (7.1) as

\[ u^n = f_1(A)b_1, \]  

(7.26)

with

\[ b_1 = \sum_{j=0}^{n-2} (b_j - b_{j+1})u^{n-1-j} + b_{n-1}u^0, \]

where \( A \) is either generated using the finite difference method (7.9) or the finite element method (7.20), \( u^0 \) is the discrete representation of the initial value \( u_0(x, y) \), \( \mu_0 \) and \( b_j \) are defined in (7.22) and (7.23), respectively.

We refer to (7.26) as Scheme 1 throughout the remaining sections of this chapter. In Section 7.3, we show how this numerical scheme can be implemented using either the Lanczos method if \( A \) is generated from the finite difference method, or the M-Lanczos method if \( A \) is generated from the finite element method.

### 7.2.4 Laplace transform method with matrix transform method

We now consider an alternative strategy for approximating the fractional differential system (7.8) associated with the TSFDE-2D (7.1). Taking the Laplace transform of (7.8) with \( \tilde{u}^n = \mathcal{L}\{u^n(t)\} \) yields

\[ s\gamma \tilde{u}^n - s^{\gamma-1}u^0 = -K_\alpha A^{\alpha/2}\tilde{u}^n, \]  

(7.27)

i.e.,

\[ \tilde{u}^n = \left[ sI + s^{1-\gamma}K_\alpha A^{\alpha/2} \right]^{-1} u^0. \]  

(7.28)

If \( A \) can be diagonalised as

\[ A = \mathbf{P} \Lambda \mathbf{P}^{-1}, \]  

(7.29)
where \( \Lambda = \text{diag}(\lambda_i, i = 1, \ldots, m) \), \( \lambda_i \) being the eigenvalues of \( A \), then from (7.28), we obtain

\[
\mathbf{u}^n = \mathcal{L}^{-1} \left\{ \left[ s \mathbf{I} + s^{1-\gamma} K_\alpha A^{\alpha/2} \right]^{-1} \mathbf{u}^0 \right\} \\
= \mathbf{P} \text{ diag} \left\{ \mathcal{L}^{-1} \left\{ \frac{1}{s + s^{1-\gamma} K_\alpha \lambda_i^{\gamma/2}} \right\}, i = 1, \ldots, m \right\} \mathbf{P}^{-1} \mathbf{u}^0. \tag{7.30}
\]

To perform the required inversion we require the Mittag–Leffler function \( E_\gamma(z) \) [116]:

\[
E_\gamma(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\gamma k + 1)}, \tag{7.31}
\]

which is a generalisation of the exponential function, with Laplace transform given by

\[
\mathcal{L} \{ E_\gamma(-\omega t) \} = \frac{s^{\gamma-1}}{s^\gamma + \omega}, \quad \Re(s) > |\omega|^{1/\gamma}. \tag{7.32}
\]

Using (7.32), we obtain

\[
\mathbf{u}^n = \mathbf{P} \text{ diag} \left\{ E_\gamma(-K_\alpha \lambda_i^{\gamma/2} t_n^{\gamma}), i = 1, \ldots, m \right\} \mathbf{P}^{-1} \mathbf{u}^0 \tag{7.33}
\]

\[
= E_\gamma(-K_\alpha A^{\alpha/2} t_n^{\gamma}) \mathbf{u}^0. \tag{7.34}
\]

Defining the scalar function \( f_2(\xi) = E_\gamma(-K_\alpha \xi^{\alpha/2} t_n^{\gamma}) \), we obtain the second numerical scheme for approximating the TSFDE-2D (7.1) as

\[
\mathbf{u}^n = f_2(A) \mathbf{b}_2, \tag{7.35}
\]

with

\[
\mathbf{b}_2 = \mathbf{u}^0.
\]

We refer to (7.35) as Scheme 2 throughout the remaining sections of this chapter. In Section 7.3, we show how this numerical scheme can be implemented using either the Lanczos method if \( A \) is generated from the finite difference method, or the M-Lanczos method if \( A \) is generated from the finite element method.
Matrix function approximation and solution strategy

In this section, we devise efficient algorithms to approximate the matrix-vector products $f_1(A)b_1$, $f_2(A)b_2$ for Schemes 1 and 2 in Sections 7.2.3 and 7.2.4, respectively.

The prevailing method in the literature for approximating the matrix-vector product $f(A)b$ for a scalar, analytic function $f(t): D \subset \mathbb{C} \rightarrow \mathbb{C}$ is the Lanczos approximation

$$f(A)b \approx \|b\|V_m f(T_m) e_1,$$

$$b = \|b\|V_m e_1,$$

(7.36)

where

$$A V_m = V_m T_m + \beta_m v_{m+1} e_m^T$$

(7.37)

is the Lanczos decomposition and the columns of $V_m$ form an orthonormal basis for the Krylov subspace $K_m(A, b) = \text{span}\{b, Ab, \ldots, A^{m-1}b\}$. This approximation has been considered by van der Vorst [145], Saad [125], Druskin & Knizhnerman [31], Hochbruck & Lubich [56], Sidje [137], van den Eshof et al. [144], Eiermann & Ernst [34], Lopez & Simoncini [93], Ilić, Turner & Anh [62] and Ilić, Turner & Simpson [63], as well as many other researchers during the last twenty years.

The standard Lanczos method requires that the matrix $A$ must be symmetric. Although the matrix $A$ generated from the finite difference method is symmetric, $A$ generated from the finite element method is non-symmetric. Therefore, we need different approximation strategies for the numerical schemes depending on the method used to generate the matrix $A$.

Lanczos method with an adaptive preconditioner

In this section, we assume the matrix $A$ is generated from the finite difference method as illustrated in Section 7.2.1, and hence is symmetric. Thus, we can use the standard Lanczos method. Memory constraints often require restarting the Lanczos decomposition; however, this is not straightforward in the context of matrix function approximation. To improve convergence of the Lanczos approximation, in this section, we use an adaptively preconditioned Lanczos method [62].
Firstly, using Lehoucq and Sorensen’s implicitly restarted Arnoldi method \cite{72}, we compute the \( k \) smallest eigenvalues \( \{\theta_i\}_{i=1}^k \) and corresponding eigenvectors \( \{q_i\}_{i=1}^k \) of the matrix \( A \). Setting \( Q_k = [q_1, q_2, \ldots, q_k] \) and \( \Lambda_k = \text{diag}\{\theta_1, \ldots, \theta_k\} \), the preconditioner \( Z^{-1} \) takes the form

\[
Z^{-1} = \theta^* Q_k \Lambda_k^{-1} Q_k^T + I - Q_k Q_k^T,
\]

where \( \theta^* = \frac{\theta_{\text{min}} + \theta_{\text{max}}}{2} \). Here \( \theta_{\text{min}}, \theta_{\text{max}} \) are the smallest and largest eigenvalues of \( A \) respectively, obtained from the implicit restarted Arnoldi process \cite{125}. This preconditioner eliminates the influence of the \( k \) smallest eigenvalues of \( A \) on the rate of convergence of the standard Lanczos method. The matrix \( A Z^{-1} \) has the same eigenvectors as \( A \) however its eigenvalues \( \{\lambda_i\}_{i=1}^k \) are shifted to \( \theta^* \). [10, 37]. We now show how this spectral information can be used to aid with the approximation of \( u^n = f(A)b \).

The important observation at this point is the following relationship between \( f(A) \) and \( f(AZ^{-1}) \).

**Proposition 7.2.** \cite{62} Let \( \text{span}\{q_1, q_2, \ldots, q_k\} \) be an eigenspace of symmetric matrix \( A \) such that \( AQ_k = Q_k A_k \), with \( Q_k = [q_1, q_2, \ldots, q_k] \) and \( \Lambda_k = \text{diag}\{\theta_1, \ldots, \theta_k\} \). Define \( Z = \frac{1}{\theta^*} Q_k \Lambda_k Q_k^T + I - Q_k Q_k^T \), then for \( v \in \mathbb{R}^n \)

\[
f(A)v = Q_k f(A_k)Q_k^T v + f(AZ^{-1})(I - Q_k Q_k^T)v.
\]

Using Proposition 7.2, we can approximate \( u^n = f(A)b \) as

\[
f(A)b = Q_k f(A_k)Q_k^T b + f(AZ^{-1})\hat{b}, \tag{7.38}
\]

where \( \hat{b} = (I - Q_k Q_k^T)b \). Note that if \( A \) is symmetric positive definite then so too is \( AZ^{-1} \).

Hence, we can apply the standard Lanczos decomposition to \( AZ^{-1} \), i.e.,

\[
AZ^{-1} V_m = V_m T_m + \beta_m v_{m+1} e_m^T,
\]

where \( v_1 = \hat{b}/\|\hat{b}\| \). Next perform the spectral decomposition of \( T_m = Y_m \tilde{\Lambda}_m Y_m^T \) and set \( \tilde{Q}_m = V_m Y_m \), then compute the Lanczos approximation

\[
f(AZ^{-1})\hat{b} \approx V_m f(T_m) V_m^T \hat{b} = \tilde{Q}_m f(\tilde{\Lambda}_m) \tilde{Q}_m^T \hat{b}. \tag{7.39}
\]
Based on the theory presented to this point, we propose the following algorithm to approximate the solution of the TSFDE-2D (7.1).

**Input:** Discretise Laplacian matrix $A$, right hand side vector $b$, tolerance $\tau$, order of spatial derivative $\alpha$, order of temporal derivative $\gamma$, number of time steps $n$, number of stored Ritz pairs $k$, and maximum size of Krylov subspace $\text{maxiter}$.

**Output:** $u^n$

Compute $\Lambda_k$ and $Q_k$ to construct preconditioner $Z^{-1}$;

for time step $j=1:n$ do
  Set $\omega = (I - Q_kQ_k^T)b$;
  Set $v_1 = \omega/\|\omega\|_2$;
  for $m = 1 : \text{maxiter}$ do
    Set $q = AZ^{-1}v_m$;
    if $m \neq 1$ then
      $q = q - \beta_{m-1}v_{m-1}$;
    end
    $\alpha_m = v_m^Tv_m$;
    $q = q - \alpha_m v_m$;
    $\beta_m = \|q\|_2$;
    $v_{m+1} = q/\beta_m$;
  end
  Compute linear system residual $\|r_m\|_2 = \|\omega\|_2 \|\beta_m e_m^T T_m^{-1} e_1\|$;
  Compute $\mu_{\text{min}}$ – the smallest eigenvalue of $T_m$;
  For Scheme 1, compute error bound as $f(\mu_{\text{min}})\|r_m\|_2$;
  For Scheme 2, compute error bound as $\frac{1}{\pi} \int_0^\infty \frac{|\Im E_\gamma(\cdot)| e^{\mu_{\text{min}}/2} e^{i\alpha/2} e^{\gamma t / 2} d\zeta}{\mu_{\text{min}} + \zeta} \|r_m\|_2$;
  if $\text{error bound} < \tau$ then
    break;
  end
  Compute $u^j = Q_kf(\Lambda_k)Q_k^T b + \|\omega\|_2 V_m f(T_m)e_1$;
end

**Algorithm 7.1:** Lanczos approximation to $f_1(A)b_1$, $f_2(A)b_2$ with adaptive preconditioning, where $A$ is symmetric positive definite.

**Remark 7.1.** In Algorithm 7.1, the preconditioner $Z^{-1}$ does not need to be explicitly formed, since it can be applied in a straightforward manner from the stored locked Ritz pairs $Q_k$ and $\Lambda_k$. These matrices are computed using MATLAB’s `eigs` function.

**Remark 7.2.** In Algorithm 7.1, the error bounds for approximating $f_1(A)b_1$, $f_2(A)b_2$, where $A \in \text{SPD}$, are derived in Section 7.3.3. To compute the error bound for Scheme 2, one needs to approximate an indefinite integral for a given time. To do this, we first evaluate $|\Im E_\gamma(\cdot)|$ in the integrand using the MATLAB code `mlf.m` developed by Podlubny. The integral
7.3 Matrix function approximation and solution strategy

is then computed using MATLAB’s \texttt{quadgk} function, which is developed based on the adaptive Gauss-Kronrod quadrature formula and allows the case where the integral limit is infinity to be evaluated. Our findings from numerical experimentation indicate that when $\alpha + \gamma \geq 2$ convergence issues arise with the evaluation of $E_{\gamma}(\cdot)$. Similar problems are also discussed in [46]. We have proved that absolute convergence of the integral in the Stieltjes transform requires that $\alpha + \gamma < 2$. Whether other possibilities hold needs further investigation, which we intend to pursue in future research.

**Remark 7.3.** In Algorithm 7.1, the smallest eigenvalue $\lambda_{\min}$ of $AZ^{-1}$ is approximated by the smallest eigenvalue $\mu_{\min}$ of $T_m$.

### 7.3.2 M-Lanczos method with an incomplete Cholesky preconditioner

In Section 7.2.1.2, we saw that the approximate matrix representation of the Laplacian corresponding to the finite element method was non-symmetric. In this section, we investigate the matrix function approximations based on the Arnoldi decomposition in the $M$–inner product $\langle x, y \rangle_M = x^T My$. The $M$–Arnoldi decomposition is well-known in the context of solving non-symmetric linear systems [138]. Essai [40] showed that the $M$–Arnoldi decomposition is of the form

$$A \tilde{V}_m = \tilde{V}_m H_m + \tilde{\beta}_m \tilde{v}_{m+1} e_m^T,$$

where the columns of $\tilde{V}_m$ form a basis for $\mathcal{K}_m(A, b)$, $\tilde{V}_m^T M \tilde{V}_m = I$ and $H_m = \tilde{V}_m^T MA \tilde{V}_m$ is an $m \times m$ upper Hessenberg matrix.

The advantage of using the $M$–inner product is that, as $A$ is $M$-self-adjoint, $H_m$ is a symmetric tridiagonal matrix and the $M$-Arnoldi decomposition can be replaced with the $M$-Lanczos decomposition

$$A \tilde{V}_m = \tilde{V}_m T_m + \tilde{\beta}_m \tilde{v}_{m+1} e_m^T.$$

Using the $M$-Lanczos decomposition, we can define the $M$-Lanczos approximation to $f(A)b$
as
\[ f(A)b \approx \|b\|_M \tilde{V}_m f(\tilde{T}_m)e_1, \]  
(7.40)

where \( \|b\|_M = \sqrt{(b,b)_M} \).

The algorithm for the M-Lanczos decomposition is given in Algorithm 7.2, which is identical to the standard Lanczos approximation with every norm and inner product replaced with the M–norm and the M–inner product.

**Input:** Mass matrix \( M \), Stiffness matrix \( K \), right hand side vector \( S \) \( b \), tolerance \( \tau \), order of spatial derivative \( \alpha \), order of temporal derivative \( \gamma \), number of time steps \( n \), and maximum size of Krylov subspace \( \text{maxiter} \).

**Output:** \( u^n \)

**Algorithm 7.2:** M–Lanczos approximation to \( f_1(M^{-1}K)b_1 \), \( f_2(M^{-1}K)b_2 \), where \( M \) and \( K \) are symmetric positive definite matrices.

**Remark 7.4.** In Algorithm 7.2, the evaluation of \( M^{-1}K\tilde{v}_m \) is done by solving \( Mq = K\tilde{v}_m \).
using the conjugate gradient method preconditioned with an incomplete Cholesky factorisation. We use MATLAB functions \texttt{pcg} and \texttt{cholinc} for this purpose.

**Remark 7.5.** In Algorithm 7.2, the error bounds for approximating \( f_1(A)b_1, f_2(A)b_2 \), where \( A = M^{-1}K \) is non-symmetric, are derived in Section 7.3.3. The numerical evaluation of the integral in the error bound for Scheme 2 is discussed in Remark 7.2.

**Remark 7.6.** In Algorithm 7.2, \( \kappa_2(M^{\frac{1}{2}}) \) is the 2-norm condition number of \( M^{\frac{1}{2}} \), computed using Matlab’s\texttt{condest} function.

**Remark 7.7.** In Algorithm 7.2, the smallest eigenvalue \( \theta_{\min} \) of \( A \) can be either computed using MATLAB’s\texttt{eigs} function, or taken as \( \theta_{\min} = 2\pi^2 \), which is an approximation of the smallest eigenvalue of the Laplacian operator [35].

### 7.3.3 Error bounds for the numerical solution

In this section, we derive the error bounds used in Algorithms 7.1 and 7.2 for the two new numerical methods and illustrate their roles in solving the TSFDE-2D (7.1).

Firstly, we will show that both functions \( f_k \ (k = 1, 2) \) can be written in the form

\[
f_k(\xi) = \int_0^\infty \frac{g_k(\zeta)d\zeta}{\xi + \zeta}, \quad \xi > 0,
\]

(7.41)

such that \( \int_0^\infty \frac{g_k(\zeta)d\zeta}{\xi + \zeta} \) is absolutely integrable. Eq.(7.41) is known as a Stieltjes integral equation [36].

When \( A \in SPD \), the following proposition gives the error in approximating \( f_k(A)b \ (k = 1, 2) \) by the Lanczos approximation (7.36) when \( f_k(\xi) \) is expressable in the form (7.41). In this section, unless otherwise stated, \( \| \cdot \| \) represents the 2-norm.

**Proposition 7.3.** Define \( r_m \) as the residual in solving \( Ax = b \) using \( m \) steps of the full orthogonalization method (FOM) [126], then

\[
\varepsilon_m^{(k)} := f_k(A)b - \|b\|V_m f_k(T_m)e_1
= \int_0^\infty g_k(\zeta) (A + \zeta I)^{-1} \left( \frac{e^T_m(T_m + \zeta I_m)^{-1}e_1}{e^T_m T_m^{-1} e_1} \right) r_m d\zeta.
\]
Proof.

\[ f_k(A) b - \|b\| V_m f_k(T_m) e_1 \]
\[ = \int_0^\infty g_k(\zeta) \left\{ (A + \zeta I)^{-1} b - \|b\| V_m(T_m + \zeta I_m)^{-1} e_1 \right\} d\zeta \]
\[ = \int_0^\infty g_k(\zeta) (A + \zeta I)^{-1} \left\{ b - \|b\| V_m e_1 - \|b\| \beta_m v_{m+1} e^T_m (T_m + \zeta I_m)^{-1} e_1 \right\} d\zeta \]
\[ = -\|b\| \beta_m \int_0^\infty g_k(\zeta) (A + \zeta I)^{-1} \left( e^T_m (T_m + \zeta I_m)^{-1} e_1 \right) v_{m+1} d\zeta \]
\[ = \int_0^\infty g_k(\zeta) (A + \zeta I)^{-1} \left( \frac{e^T_m (T_m + \zeta I_m)^{-1} e_1}{e^T_m T_m e_1} \right) \left( -\|b\| \beta_m (e^T_m T_m^{-1} e_1) v_{m+1} \right) d\zeta \]
\[ = \int_0^\infty g_k(\zeta) (A + \zeta I)^{-1} \left( \frac{e^T_m (T_m + \zeta I_m)^{-1} e_1}{e^T_m T_m^{-1} e_1} \right) r_m d\zeta, \]

where \( r_m = -\|b\| \beta_m (e^T_m T_m^{-1} e_1) v_{m+1}. \) \( \square \)

Note that if \( A \in SPD \) then \( AZ^{-1} \in SPD, \) where \( Z^{-1} \) is discussed in Section 7.3.1. Thus, \( AZ^{-1} \) can be orthogonally diagonalised with its smallest eigenvalue \( \lambda_{\text{min}}, \) and using the result from Ilić, Turner & Anh [62] that

\[ \left| \frac{e^T_m (T_m + \zeta I_m)^{-1} e_1}{e^T_m T_m^{-1} e_1} \right| < 1, \]

the error bound for the Lanczos approximation (7.39) can be written as

\[ \|\varepsilon^{(k)}_m\| \leq \int_0^\infty \frac{|g_k(\zeta)|}{\lambda_{\text{min}} + \zeta} \|r_m\| \, d\zeta, \quad k = 1, 2. \]

In the case where \( A = M^{-1} K \) is positive definite (see Proposition 7.1) and \( f_k(\xi) \) is expressed in the form (7.41), we have the following proposition for defining the error in approximating \( f_k(A)b \) \( (k = 1, 2) \) by the M-Lanczos approximation (7.40).

**Proposition 7.4.** Define \( \tilde{r}_m \) as the residual in solving \( Ax = b \) using M-weighted FOM [40] by \( \tilde{r}_m = -\|b\| \beta_m (e^T_m T_m^{-1} e_1) \tilde{v}_{m+1}, \) then

\[ \varepsilon^{(k)}_m := f_k(A)b - \|b\| M \tilde{V}_m f_k(T_m) e_1 \]
\[ = \int_0^\infty g_k(\zeta) (A + \zeta I)^{-1} \left( \frac{e^T_m (T_m + \zeta I_m)^{-1} e_1}{e^T_m T_m^{-1} e_1} \right) \tilde{r}_m d\zeta. \]
Proof. Proceeding as in Proposition 7.3, we have

\[ f_k(A)b - \|b\|_M \tilde{V}_m f_k(\tilde{T}_m)e_1 \]
\[ = - \|b\|_M \tilde{\beta}_m \int_0^\infty g_k(\zeta)(A + \zeta I)^{-1} \left( e^T_m(\tilde{T}_m + \zeta I_m)^{-1}e_1 \right) \tilde{v}_{m+1} \, d\zeta \]
\[ = \int_0^\infty g_k(\zeta) (A + \zeta I)^{-1} \left( e^T_m(\tilde{T}_m + \zeta I_m)^{-1}e_1 \right) e_1 \, d\zeta. \]

We now show that \( A = M^{-1}K \) is diagonalisable. First recall from Proposition 7.1 that \( A \) is similar to the SPD matrix \( \tilde{A} = M^{-\frac{1}{2}}KM^{-\frac{1}{2}} \). Thus, \( \tilde{A} \) can be orthogonally diagonalised as \( \tilde{A} \tilde{P} = \tilde{P} \Lambda \) and therefore \( M^{-\frac{1}{2}} \tilde{A} \tilde{P} = M^{-\frac{1}{2}} \tilde{P} A \), which implies that \( M^{-1}K(M^{-\frac{1}{2}} \tilde{P}) = (M^{-\frac{1}{2}} \tilde{P})A \). Thus \( A = \tilde{P} \Lambda \tilde{P}^{-1} \), where \( \tilde{P} = M^{-\frac{1}{2}} \tilde{P} \), \( P = M^{-\frac{1}{2}} \tilde{P} \), \( P^{-1} = \tilde{P}^T M^\frac{1}{2} \).

Hence, we have the error bound for the M-Lanczos approximation (7.40)

\[ \|\tilde{e}^{(k)}_m\| \leq \kappa_2(M^\frac{1}{2}) \int_0^\infty \frac{|g_k(\zeta)|}{\theta_{\text{min}} + \zeta} \|\tilde{r}_m\| \, d\zeta, \quad k = 1, 2, \]

where \( \kappa_2(M^\frac{1}{2}) = \sqrt{\mu^*_{\text{max}}/\mu^*_{\text{min}}} \) is the condition number of \( M^\frac{1}{2} \), with \( \mu^*_{\text{max}} \) and \( \mu^*_{\text{min}} \) are the largest and smallest eigenvalues of \( M \) respectively; and \( \theta_{\text{min}} \) is the smallest eigenvalue of \( A = M^{-1}K \).

One method of solution for the Stieltjes integral equation (7.41) is possible if \( f_k(\xi) \) is analytic with a cut on the negative real axis, in which case [36]

\[ g_k(\zeta) = \frac{i}{2\pi} \left\{ f_k(\zeta e^{i\pi}) - f_k(\zeta e^{-i\pi}) \right\}, \quad k = 1, 2. \]  

(7.42)

Proposition 7.5. For numerical Scheme 1, \( f_1(\xi) = \left[1 + \mu_0 K_0 \xi^{\alpha/2}\right]^{-1} \) with \( \xi > 0, \mu_0 > 0, \]
\( K_0 > 0, 1 < \alpha \leq 2 \), we obtain

\[ g_1(\zeta) = \frac{\mu_0 K_0 \sin(\frac{\pi \alpha}{2})}{\pi}, \quad \frac{\zeta^{\alpha/2}}{1 + 2\mu_0 K_0 \zeta^{\alpha/2} \cos(\frac{\pi \alpha}{2}) + (\mu_0 K_0 \zeta^{\alpha/2})^2} \]

and

\[ f_1(\xi) = \frac{\mu_0 K_0 \sin(\frac{\alpha \pi}{2})}{\pi} \int_0^\infty \frac{\zeta^{\alpha/2} \, d\zeta}{(1 + 2\mu_0 K_0 \zeta^{\alpha/2} \cos(\frac{\pi \alpha}{2}) + (\mu_0 K_0 \zeta^{\alpha/2})^2)(\xi + \zeta)}. \]
Proof. Clearly \( f_1(\xi) \) is analytic with cut \((-\infty, 0]\). From (7.42),

\[
g_1(\zeta) = \frac{i}{2\pi} \left\{ \frac{1}{1 + \mu_0 K_0 \zeta^{\alpha/2} e^{i\pi \alpha/2}} - \frac{1}{1 + \mu_0 K_0 \zeta^{\alpha/2} e^{-i\pi \alpha/2}} \right\}
\]

\[
= \frac{i}{2\pi} \cdot \frac{\mu_0 K_0 \zeta^{\alpha/2} [1 - 2i \sin(\frac{\pi \alpha}{2})]}{1 + 2\mu_0 K_0 \zeta^{\alpha/2} \cos(\frac{\pi \alpha}{2}) + (\mu_0 K_0 \zeta^{\alpha/2})^2}
\]

\[
= \frac{\mu_0 K_0 \sin(\frac{\pi \alpha}{2})}{\pi} \cdot \frac{\zeta^{\alpha/2}}{1 + 2\mu_0 K_0 \zeta^{\alpha/2} \cos(\frac{\pi \alpha}{2}) + (\mu_0 K_0 \zeta^{\alpha/2})^2}.
\]

Hence, we have

\[
f_1(\xi) = \frac{\mu_0 K_0 \sin(\frac{\pi \alpha}{2})}{\pi} \int_0^{\infty} \frac{\zeta^{\alpha/2} d\zeta}{(1 + 2\mu_0 K_0 \zeta^{\alpha/2} \cos(\frac{\pi \alpha}{2}) + (\mu_0 K_0 \zeta^{\alpha/2})^2)(\xi + \zeta)}.
\]

Interestingly, Alzer and Berg [4] state that a function \( f \) is a Stieltjes transform if (i) \( f \) is holomorphic in the cut plane \( \mathcal{A} = \mathbb{C} \setminus (-\infty, 0] \); (ii) satisfies \( \Im f(z) \leq 0 \) for \( \Im z > 0 \); and (iii) \( f(\xi) \geq 0 \) for \( \xi > 0 \). Furthermore, the measure is given by \( d\mu(\zeta) = g(\zeta) d\zeta \), where \( \mu \) is the limit in the vague topology of measures and \( g(\zeta) = -\frac{1}{\pi} \lim_{y \to 0^+} \Im f(-\zeta + iy) \). Clearly,

\[
f_1(\xi) = \frac{1}{1 + \mu_0 K_0 \xi^{\alpha/2}} \text{ where } \mu > 0, K_0 > 0 \text{ and } 1 < \alpha \leq 2 \text{ has a branch cut } (-\infty, 0] \text{ and for the principal branch } -\pi < \arg(\xi) \leq \pi \text{ this function has no singularities, and hence condition (i) holds. Also, (iii) holds and condition (ii) also holds, since for } z = re^{i\theta}, 0 < \theta < \pi, \text{ we have}
\]

\[
\Im f_1(z) = \frac{-\mu_0 K_0 r^{\alpha/2} \sin(\frac{\pi \alpha}{2})}{(1 + \mu_0 K_0 r^{\alpha/2} \cos(\frac{\pi \alpha}{2}))^2 + \mu_0^2 K_0^2 r^{\alpha} \sin^2(\frac{\pi \alpha}{2})} \leq 0.
\]

We conclude that \( f_1(\xi) \) is a Stieltjes transform. In this case, using Theorem 5.4 in Ilić et al. [63] we obtain the error bound for the Lanczos approximation (7.39) using Scheme 1,

\[
\|e_m^{(1)}\| \leq f_1(\lambda_{min}) \|r_m\|,
\]

where \( \lambda_{min} \) is the smallest eigenvalue of \( A Z^{-1} \). It also follows that the error bounds for the M-Lanczos approximation (7.40) using Scheme 1 is given by

\[
\|\tilde{e}_m^{(1)}\| \leq \kappa_2(M^2) f_1(\theta_{min}) \|\tilde{r}_m\|,
\]

where \( \theta_{min} \) is the smallest eigenvalue of \( A \).

We now derive an error bound for \( f_2(\xi) \) using the same strategies as those outlined above. We
begin with the following proposition.

**Proposition 7.6.** For numerical Scheme 2, \( f_2(\xi) = E_\gamma(-K_\alpha \xi^{\alpha/2} t_n^\gamma) \) with \( \xi > 0, K_\alpha > 0, 1 < \alpha \leq 2 \), we obtain

\[
g_2(\zeta) = -\frac{1}{\pi} \Im E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2})
\]

and

\[
f_2(\xi) = -\frac{1}{\pi} \int_0^\infty \frac{\Im E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2})}{\xi + \zeta} d\zeta.
\]

**Proof.** First recall from (7.31) that \( E_\gamma(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\gamma k + 1)} \). Clearly \( f_2(\xi) \) is analytic with cut \((-\infty, 0]\), and from (7.42)

\[
g_2(\zeta) = \frac{i}{2\pi} \left\{ E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2}) - E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{-i\pi \alpha/2}) \right\}
\]

\[
= \frac{i}{2\pi} \sum_{k=0}^{\infty} \left( -K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2} \right)^k \cdot \frac{2i \sin\left(\frac{k\pi}{2}\right)}{\Gamma(1 + \gamma k)}
\]

\[
= -\frac{1}{\pi} \Im \sum_{k=0}^{\infty} \left( -K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2} \right)^k \frac{1}{\Gamma(1 + \gamma k)}
\]

\[
= -\frac{1}{\pi} \Im E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2}).
\]

Hence,

\[
f_2(\xi) = -\frac{1}{\pi} \int_0^\infty \Im E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2}) d\zeta. \tag*{□}
\]

To proceed we must bound \( |g_2(\zeta)| = \left| \frac{1}{\pi} \Im E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2}) \right| \). Theorem 1.6 in Podlubny’s book [116] suggests that there exists a real constant \( C \) such that \( E_\gamma(z) \leq \frac{C}{1 + |z|} \) provided \( \frac{\pi \gamma}{2} < \arg(z) < \pi, |z| \geq 0 \). Thus, we have

\[
|g_2(\zeta)| = \frac{1}{\pi} \left| \Im E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2}) \right| \leq \frac{\left| E_\gamma(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2}) \right|}{\pi}
\]

\[
\leq \frac{C}{\pi(1 + K_\alpha \zeta^{\alpha/2} t_n^\gamma)},
\]

provided \( \frac{\pi \gamma}{2} < |\arg(-K_\alpha \zeta^{\alpha/2} t_n^\gamma e^{i\pi \alpha/2})| \leq \pi \), which necessitates \( \frac{\gamma}{2} < 1 - \frac{\alpha}{2} \leq 1 \). Hence, we require \( \alpha + \gamma < 2 \) with \( 1 < \alpha \leq 2 \) and \( 0 < \gamma < 1 \).
Thus, the error bound for the Lanczos approximation (7.39) using Scheme 2 is given as
\[ \|\varepsilon_{m}^{(2)}\| \leq \frac{1}{\pi} \int_{0}^{\infty} \left| \Im \left( E_{\gamma}(-K_{\alpha}^{\alpha/2}t_{n}^{\gamma}e^{i\pi\alpha/2}) \right) \right| d\gamma \lambda_{\min} + \zeta \|r_{m}\|, \] (7.43)
where \(\lambda_{\min}\) is the smallest eigenvalue of \(AZ^{-1}\). Also, the error bound for the M-Lanczos approximation (7.40) using Scheme 2 is given by
\[ \|\tilde{\varepsilon}_{m}^{(2)}\| \leq \kappa_{2}(M_{1}^2) \int_{0}^{\infty} \left| \Im \left( E_{\gamma}(-K_{\alpha}^{\alpha/2}t_{n}^{\gamma}e^{i\pi\alpha/2}) \right) \right| d\gamma \theta_{\min} + \zeta \|\tilde{r}_{m}\|, \] (7.44)
where \(\theta_{\min}\) is the smallest eigenvalue of \(A\).

7.4 Analytical solution of the homogeneous TSS-FKE in 2-D

In this section, we derive the analytical solution of the homogeneous TSFDE-2D with homogeneous Dirichlet boundary conditions on the rectangular domain \([0, a] \times [0, b]\\):

\[ tD_{x}^{\gamma}u(x, y, t) = -K_{\alpha}(-\Delta)^{\alpha/2}u(x, y, t), \] (7.45)
\[ u(0, y, t) = u(a, y, t) = 0, \] (7.46)
\[ u(x, 0, t) = u(x, b, t) = 0, \] (7.47)
\[ u(x, y, 0) = u_{0}(x, y), \] (7.48)

with \(0 < \gamma < 1, 1 < \alpha \leq 2\).

Now set \(u(x, y, t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_{n,m}(t)\varphi_{n,m}\\). Using Definition 7.1 and substituting \(u(x, y, t)\\) into (7.45), we obtain
\[ \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} tD_{x}^{\gamma}c_{n,m}(t)\varphi_{n,m} = -K_{\alpha} \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_{n,m}(t)(\lambda_{n,m})^{\alpha/2}\varphi_{n,m}, \] (7.49)
i.e.
\[ tD_{x}^{\gamma}c_{n,m}(t) = -K_{\alpha}c_{n,m}(t)(\lambda_{n,m})^{\alpha/2}. \] (7.50)
7.4 Analytical solution of the homogeneous TSS-FKE in 2-D

Since $u(x, y, t)$ must also satisfy the initial condition (7.48)

$$\sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_{n,m}(0) \varphi_{n,m} = u_0(x, y), \quad 0 \leq x \leq a, \quad 0 \leq y \leq b, \quad (7.51)$$

we obtain

$$c_{n,m}(0) = \frac{2}{a} \frac{2}{b} \int_0^a \int_0^b u_0(x, y) \varphi_{n,m} \, dy \, dx. \quad (7.52)$$

For each value of $n$ and $m$, (7.50) and (7.52) comprise a two-dimensional fractional initial value problem. Applying the Laplace transform to (7.50), we obtain

$$s^\gamma \tilde{c}_{n,m}(s) - s^{\gamma-1} c_{n,m}(0) = -K_\alpha(\lambda_{n,m})^{\alpha/2} \tilde{c}_{n,m}(s), \quad (7.53)$$

i.e.

$$\tilde{c}_{n,m}(s) = \frac{s^{\gamma-1} c_{n,m}(0)}{s^\gamma + K_\alpha(\lambda_{n,m})^{\alpha/2}} \quad (7.54)$$

By using the known Laplace transform of the Mittag-Leffler function [116]

$$\mathcal{L} \{ E_\gamma(-\omega t^\gamma) \} = \frac{s^{\gamma-1}}{s^\gamma + \omega}, \quad \Re(s) > |\omega|^{1/\gamma}, \quad (7.55)$$

we obtain

$$c_{n,m}(t) = E_\gamma(-K_\alpha(\lambda_{n,m})^{\alpha/2} t^\gamma) c_{n,m}(0). \quad (7.56)$$

Hence, the analytic solution of the two-dimensional homogeneous TSS-FKE with homogeneous Dirichlet boundary conditions is given by

$$u(x, y, t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} c_{n,m}(t) \varphi_{n,m}$$

$$= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} E_\gamma(-K_\alpha(\lambda_{n,m})^{\alpha/2} t^\gamma) c_{n,m}(0) \varphi_{n,m}. \quad (7.57)$$


7.5 Numerical examples

**Example 1** Consider the following TSFDE-2D with homogeneous Dirichlet boundary conditions:

\[
\begin{align*}
\dot{D}_t^\gamma u(x, y, t) &= -(-\Delta)^{\alpha/2} u(x, y, t), \\
u(0, y, t) &= u(1, y, t) = 0, \\
u(x, 0, t) &= u(x, 1, t) = 0, \\
u(x, y, 0) &= xy(1-x)(1-y).
\end{align*}
\]

(7.58)

According to the derivation in Section 7.4, the analytical solution of the TSFDE-2D (7.58)–(7.61) is given by

\[
u(x, y, t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} E_{\alpha/2} \left( -\lambda_{n,m}^\gamma t^{\gamma} \right) c_{n,m}(0) \varphi_{n,m}.
\]

(7.62)

where

\[
\begin{align*}
\lambda_{n,m} &= n^2 \pi^2 + m^2 \pi^2, \\
\varphi_{n,m} &= \sin(n\pi x) \sin(m\pi y), \\
c_{n,m}(0) &= 4 \int_0^1 \int_0^1 xy(1-x)(1-y) \varphi_{n,m} \, dy \, dx.
\end{align*}
\]

(7.63)

(7.64)

(7.65)

In Figure 7.1 we illustrate the effect of the fractional order in time for this problem, with \(\alpha\) fixed at 2. The diffusion process with \(0 < \gamma < 1\) is called the subdiffusion process [71, 131, 54]. We observe the faster rate of diffusion associated with the subdiffusion process, as compared to the standard diffusion.

In Figure 7.2 we illustrate the effect of the fractional order in space for this problem, with \(\gamma\) fixed at 1. The diffusion process with \(1 < \alpha < 2\) is called the Lévy flight. We observe the slower rate of diffusion associated with the Lévy flight, as compared to the standard diffusion.

Because Scheme 2 is exact in time, all of the error in this scheme is associated with the spatial discretisation. To identify the order of convergence in space for Scheme 2, we compute the error in the numerical solution at \(t = 0.01\) with \(\alpha = 1.3\), and \(\gamma = 0.5\) for a sequence of refined
Table 7.1: Spatial errors at \( t = 0.01 \) using scheme 2 with \( \alpha = 1.3 \) and \( \gamma = 0.5 \)

<table>
<thead>
<tr>
<th>( h )</th>
<th>FDM</th>
<th>FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>6.4294e-005</td>
<td>2.2014e-004</td>
</tr>
<tr>
<td>0.05</td>
<td>1.6289e-005</td>
<td>6.3283e-005</td>
</tr>
<tr>
<td>0.025</td>
<td>4.0930e-006</td>
<td>1.5994e-005</td>
</tr>
<tr>
<td>0.0125</td>
<td>1.0264e-006</td>
<td>4.2674e-006</td>
</tr>
<tr>
<td>0.00625</td>
<td>2.6016e-007</td>
<td>1.0331e-006</td>
</tr>
<tr>
<td>Order</td>
<td>2.0</td>
<td>1.9</td>
</tr>
</tbody>
</table>

Table 7.2: Temporal errors at \( t = 0.01 \) using scheme 1 with \( h = 0.00625, \alpha = 1.3 \) and \( \gamma = 0.5 \)

<table>
<thead>
<tr>
<th>( \tau )</th>
<th>FDM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.001</td>
<td>4.8872e-004</td>
</tr>
<tr>
<td>0.0005</td>
<td>2.3559e-004</td>
</tr>
<tr>
<td>0.0025</td>
<td>1.1354e-004</td>
</tr>
<tr>
<td>0.00125</td>
<td>5.6336e-005</td>
</tr>
<tr>
<td>0.000625</td>
<td>2.7265e-005</td>
</tr>
<tr>
<td>Order</td>
<td>1.0</td>
</tr>
</tbody>
</table>

meshes. In Table 7.1, we present the \( \ell^\infty \)-norm error for both FDM and FEM. For FDM, uniform grids with grid spacing \( h \) were used. For FEM, unstructured triangular meshes with maximum element edge length \( h \) were used. The order of convergence in space for Scheme 2 is estimated to be \( O(h^2) \) for FDM and \( O(h^{1.9}) \) for FEM.

To identify the order of convergence in time for Scheme 1, we compute the error in the numerical solution at \( t = 0.01 \) using FDM on the finest mesh with \( h = 0.00625, \alpha = 1.3, \) and \( \gamma = 0.5 \). In Table 7.2, we present the \( \ell^\infty \)-norm error. The order of convergence in time for Scheme 1 is estimated to be \( O(\tau) \).

Figure 7.3 is generated using Scheme 1 with the adaptively preconditioned Lanczos method for the test problem with \( t_{final} = 1, \tau = 0.02, h = 0.05, \gamma = 0.8, \alpha = 1.3 \). In this figure, we illustrate the impact of the preconditioner on the size of the Krylov subspace \( m \) when \( k \) smallest approximate eigenpairs are used. This includes the case where \( k = 0 \), where no preconditioning was applied. We see that the average subspace size \( m \) is reduced as we increase the number of eigenpairs from \( k = 1 \) to \( k = 20 \). In Figure 7.4, we see a similar impact of the preconditioner on the subspace size \( m \) for the same test problem using Scheme 2. Another observation that can be made from these figures is that as time evolves the size of the subspace \( m \) is reduced.
Figure 7.1: Effect of fractional order in time

\[ t = 0.001, \gamma = 1 \]
\[ t = 0.001, \gamma = 0.8, \]
\[ t = 0.001, \gamma = 0.5 \]

\[ t = 0.002, \gamma = 1 \]
\[ t = 0.002, \gamma = 0.8, \]
\[ t = 0.002, \gamma = 0.5 \]

\[ t = 0.005, \gamma = 1 \]
\[ t = 0.005, \gamma = 0.8, \]
\[ t = 0.005, \gamma = 0.5 \]
7.5 Numerical examples

Figure 7.2: Effect of fractional order in space

Figure 7.3: Subspace size \( m \) at each time step for \( t_{\text{final}} = 1 \) with \( \tau = 0.02, h = 0.05, \gamma = 0.8, \alpha = 1.3 \) (Scheme 1 using the adaptively preconditioned Lanczos method)
Chapter 7. Novel numerical methods for solving TSFDE-2D

7.6 Conclusions

In this paper, we derived two novel numerical methods to solve the TSFDE-2D. We demonstrated how either the finite difference or finite element methods can be used for the discretisation in space and how the finite difference method or the Laplace transform method can be used for the time advancement of the solution. We investigated both the Lanczos and M-Lanczos methods for approximating the matrix function vector product $f_k(A)b_k$ ($k = 1, 2$), and highlighted the performance that preconditioning can offer in these algorithms. Error bounds were proposed to terminate the Lanczos subspace expansion. Our numerical investigation highlighted that both schemes provide accurate solutions in comparison with the derived analytical results and offer order $O(\tau + h^2)$. In conclusion, either scheme can be used, however, we recommend Scheme 2 in light of it being exact in time.
The major objective of this thesis was to develop new efficient numerical methods and supporting analysis for solving time, space, and time-space fractional dynamical systems in one and two spatial dimensions. Since the fractional derivative is a non-local operator, the classical numerical methods are not adequate to handle the fractional case, which naturally leads to the necessity of deriving new approximation techniques for fractional derivatives. A series of five published papers and one manuscript in preparation has been presented on the solution of the space fractional diffusion equation, space fractional advection-dispersion equation, time and space fractional diffusion equation, time and space fractional Fokker-Planck equation with a linear or non-linear source term, and fractional cable equation involving two time fractional derivatives, respectively. These papers comprise the bulk of Chapters 2 to 7 and form the backbone of the theory associated with the newly developed numerical methods. In the next section, we discuss the main results of this thesis in greater detail. The chapter concludes with some recommendations for future research.
8.1 Summary and Discussion

In Chapter 2 we considered a fractional partial differential equation with Riesz space fractional derivatives (FPDE-RSFD). In the literature, there are several different techniques for approximating different fractional derivatives \cite{114, 116, 129}. To avoid confusion on this issue, we remarked that it is essential to adopt the correct approximation for the corresponding definition of the fractional operator. One significant contribution made in this chapter was the illustration of how to choose different techniques for different fractional derivatives.

Meerschaert and Tadjeran \cite{106} found that the standard Grünwald approximation to discretise the fractional diffusion equation results in an unstable finite difference scheme regardless of whether the resulting finite difference method is an explicit or an implicit scheme. We presented a new and novel approach whereby the the diffusion term is approximated by the shifted Grünwald method and the advection term is approximated by the standard Grünwald method. This standard/shifted Grünwald method was presented along with the L1/L2 approximation method, as two effective numerical methods based on the link between the Riemann-Liouville and Grünwald-Letnikov fractional derivatives.

In the literature, one often sees the Riesz fractional advection-dispersion equation (RFADE) defined in terms of the fractional Laplacian operator, under the assumption that the two operators are equivalent. In Chapter 2 we clarified the relationship between these two fractional operators. We showed that under the Fourier transform definition on an infinite domain, the fractional Laplacian is indeed equivalent to the Riesz fractional derivative. However, in the literature there exists a second definition of the fractional Laplacian defined on a finite domain, using eigenfunction expansion on a finite domain. We showed that although under this definition the two operators are not equivalent, numerical methods based upon this definition can nonetheless produce useful approximations. This leads to the third method presented in the chapter, i.e., the matrix transform method (MTM), to approximate the Riesz fractional derivative.

After introducing the three numerical methods to approximate the Riesz fractional derivative, we used the fractional method of lines proposed by Liu et al. \cite{78} to transform the RFDE and RFADE into a system of time ordinary differential equations (TODEs). This TODE system
was solved using a differential/algebraic system solver (DASSL) [17]. Numerical results were presented, comparing the numerical solutions to the analytic solutions, demonstrating the effectiveness and convergence of the three numerical methods. We remarked that the methods and techniques discussed can also be applied to solve other kinds of fractional partial differential equations.

In Chapter 3 we considered a time and space-symmetric fractional diffusion equation (TSS-FDE). Depending on the fractional powers of the operators, this equation can model either subdiffusion, or the Lévy process. Hence its solution is important for describing the competition between these two anomalous diffusion processes.

Two numerical schemes were presented for solving the TSS-FDE. Both methods utilise the matrix transform method to discretise the symmetric space fractional derivative. The Caputo time fractional derivative is treated either numerically, using a finite difference method, or exactly, using a Laplace transform method. It is worthwhile mentioning that the numerical scheme using Laplace transform method, i.e., LTM-MTM, is exact in time. The error observed for LTM-MTM is only associated with the spatial discretization error.

Numerical experiments were conducted, that demonstrated the effectiveness of the two proposed schemes. Comparisons of the numerical solutions against the analytic solutions showed a good match, with the accuracy of the numerical solution increasing as the time and spatial step sizes were reduced.

In Chapter 4 we considered a time- and space-fractional Fokker-Planck equation (TSFFPE). Existing numerical methods for the solution of the TSFFPE are quite limited, and published papers on the field are sparse.

We presented three numerical methods for dealing with the Riesz space fractional derivative: the L2-approximation method, the shifted Grünwald method and the matrix transform method. The TSFFPE incorporates both a standard (non-fractional) time derivative, and a Riemann-Liouville time fractional derivative. A novel time integration strategy based on the fractional implicit trapezoidal method (FITM) was proposed, and a full description of the final scheme, in conjunction with all of the aforementioned spatial discretisation approaches, was given.

It is also worthwhile mentioning that, in comparison to the previously published results based
on the Monte Carlo simulations, our numerical methods were found to be computationally efficient, requiring only a few seconds to complete execution and output the results. Comparisons between the numerical solutions and analytic solutions for a particular test problem showed excellent agreement across all methods. Numerical results for the shifted Grünwald method were also exhibited for a second problem exhibiting noteworthy anomalous diffusion behaviours.

In Chapter 5 we extended the methods of the previous chapter to the time-space fractional Fokker-Planck equation with a nonlinear source term (TSFFPE-NST) – an equation not previously considered in the literature as far as numerical methods are concerned. Adopting the L1-approximation to discretise the Caputo time fractional derivative, and the shifted Grünwald approximation to discretise the symmetric Riesz space fractional derivative, we arrived at an effective numerical method to solve the TSFFPE-NST. Note that in the method under consideration, the nonlinear source term was handled explicitly in order to avoid the need to solve a nonlinear system at each time step. However, we also gave the form of the numerical method if an implicit scheme were to be used.

The stability of the numerical scheme was established theoretically, under the assumption that the nonlinear source term satisfies a Lipschitz condition and the drift coefficient decreases monotonically. We noted that this second assumption is supported by physical considerations. Several remarks were made on how these assumptions can be weakened, while still obtaining a stable numerical scheme. The corresponding result for the implicit handling of the source term was also remarked upon, whereby it was observed that the implicit scheme is generally stable when the time step is small.

Under the same set of assumptions we were also able to establish the convergence of the (explicit) scheme. Again, we remarked that the corresponding implicit scheme will also generally be convergent if the time step is small.

Numerical results were presented that supported the theoretical analysis. In particular, by comparing the numerical solutions to the analytic solution for a particular test problem, the errors satisfied the relationship $\text{error} \leq (\tau^{1+\alpha} + h + \tau)$ derived in the previous sections.

Further test problems were analysed in order to investigate the effect that the different terms in the TSFFPE-NST have on the solution. With appropriate choices of the fractional powers, the solution profile can be observed to exhibit a sharp peak and a heavy tail. A TSFFPE-NST with
a nonlinear source term representing Fisher’s population growth model was investigated. Interestingly, though this source term is not globally Lipschitz continuous, the numerical solution for this problem was nevertheless found to converge.

In Chapter 6, we considered the fractional cable equation – an equation of practical importance that involves two Riemann-Liouville time fractional derivatives of different orders. We derived a new implicit method for the numerical solution of this equation. Using the energy method, and introducing a new energy norm, we were able to show that the proposed method is stable. Subsequently, by defining another, new, energy norm, we were also able to show that the method is convergent, exhibiting first order accuracy in time and second order accuracy in space.

We then presented a second implicit numerical method that improves upon the first by increasing the temporal accuracy to second order. Numerical experiments were presented that support the validity of these theoretical results.

We noted that the proposed numerical techniques allow for simulation of the case where the fractional exponents of the two temporal derivatives are not equal. Results from numerical experimentation reveal that there is a crossover between more and less anomalous behaviour – another new contribution to the literature.

In Chapter 7, we derived two novel numerical methods to solve the TSFDE-2D. We demonstrated how either the finite difference or finite element methods can be used for the discretisation in space and how the finite difference method or the Laplace transform method can be used for the time advancement of the solution. We investigated both the Lanczos and M-Lanczos methods for approximating the matrix function vector product \( f_k(A)b_k \) \((k = 1, 2)\), and highlighted the performance that preconditioning can offer in these algorithms. Error bounds were proposed to terminate the Lanczos subspace expansion. Our numerical investigation highlighted that both schemes provide accurate solutions in comparison with the derived analytical results and offer order \( O(\tau + h^2) \). In conclusion, either scheme can be used, however, we recommend Scheme 2 in light of it being exact in time.
8.2 Directions for Future Research

There are a number of extensions and applications to the methods presented in this thesis that could be pursued in the future. In particular, the following areas could lead to fruitful research:

- **Numerical methods for variable-order fractional partial differential equations**
  
  The concept of variable-order fractional integration and differentiation was proposed by Lorenzo and Hartley [95, 94]. They pointed out that the behaviour of some diffusion processes in response to temperature changes may be better described using variable-order exponents in a pseudodifferential operator rather than time-varying coefficients. Ruiz-Medina, Anh and Angulo [124] introduced a class of Markov processes whose transition probability densities are defined by multifractional pseudodifferential equations on compact domains with variable local dimension. The infinitesimal generators of these Markov processes are given by the trace of strongly elliptic pseudodifferential operators of variable order on such domains. The results derived provide an extension of some existing classes of multifractional Markov processes. In particular, pseudostable processes are defined on domains with variable local dimension in this framework. However, the research on variable-order fractional partial differential equations is a new area, and numerical approximation of these equations is still at an early stage of development. Lin, Liu, Anh and Turner [75] established an equality between the variable-order Riemann-Liouville fractional derivative and its Gr"unwald-Letnikov expansion. Using this relationship, they defined and obtained some properties of the operator \((-\frac{d^2}{dx^2})^{\alpha(x,t)}\) and devised an explicit finite difference approximation scheme for a corresponding variable-order nonlinear fractional diffusion equation

\[
\frac{\partial u(x,t)}{\partial t} = B(x,t) x R^{\alpha(x,t)} u(x,t) + f(u, x, t),
\]

where \(x R^{\alpha(x,t)}\) is a generalised Riesz fractional derivative of variable order \(\alpha(x,t)\) (1 < \(\alpha(x,t)\) ≤ 2). Zhuang, Liu, Anh and Turner [167] presented explicit and implicit Euler approximations for the variable-order fractional advection-diffusion equation with a nonlinear source term and investigated the stability and convergence of the proposed methods.
8.2 Directions for Future Research

- **The extension of the MTM, where the matrix can also be generated from the finite volume method or a meshfree method**

In Chapter 7, we have shown that, to solve the TSFDE-2D, we first introduce a mesh and discretise in space using either the finite difference or finite element methods to obtain an approximate matrix representation $A$ of the Laplacian $(-\Delta)$. Then using the MTM proposed by Ilic et al. [61], the TSFDE-2D is transformed into a system of fractional-in-time differential equations involving the matrix $A$ raised to the fractional index $\alpha/2$ as

$$\mathcal{D}_t^{\alpha} u = -K_\alpha A^{\alpha/2} u.$$ 

In summary, this MTM enables the classical numerical methods, such as finite difference/element/volume methods, and meshfree methods, to be used for the spatial discretisation of the fractional derivative. Hence, it would be interesting to consider the use of the finite volume method and meshfree methods to obtain the matrix $A$. It would also be interesting and challenging to generalise these results to higher dimensional problems, e.g. 3-D problems.

- **Applications of fractional derivatives in financial markets**

One of the new applications of fractional order models has been recently found in the description of the probability distributions of log-prices in the long-time limit, which is useful to characterise the natural variability in prices in the long term. For example, Meerschaert and Scalas [104] introduced a time-space fractional diffusion equation

$$\frac{\partial^\alpha p}{\partial t^\alpha} = D \frac{\partial^\beta p}{\partial |x|^\beta} + \delta(x)t^{-\beta}/\Gamma(1-\beta)$$

to model the CTRW scaling limit process densities when the waiting times and the log-returns are uncoupled (independent), and a coupled fractional diffusion equation

$$\left(\frac{\partial}{\partial t} - \frac{\partial^\alpha}{\partial |x|^\alpha}\right)^\beta p(x,t) = \delta(x)t^{-\beta}/\Gamma(1-\beta)$$

if the waiting times and the log-returns are coupled (dependent). The numerical techniques presented in this thesis can be applied to solve these fractional equations more efficiently, in comparison to the Monte Carlo simulation.
• Applications of anomalous diffusion in medical imaging analysis

Recently, Hall and Barrick [53] pointed out that the model of restricted diffusion commonly employed in the analysis of diffusion MR data is not valid in complex environments, such as human brain tissue. They described an imaging method based on the theory of anomalous diffusion and showed that images based on environmental complexity may be constructed from diffusion-weighted MR images, where the anomalous exponent $\gamma < 1$ and fractal dimension $dw$ were measured from diffusion-weighted MRI data. The numerical techniques that have been presented in this thesis would be suitable for use in this important application.


