

Kolade M. Owolabi  
Abdon Atangana

# Numerical Methods for Fractional Differentiation

# Springer Series in Computational Mathematics

Volume 54

## Series Editors

Randolph E. Bank, Department of Mathematics, University of California, San Diego, La Jolla, CA, USA

Ronald L. Graham, Department of Computer Science & Engineering, University of California, San Diego, La Jolla, CA, USA

Wolfgang Hackbusch, Max-Planck-Institut für Mathematik in den Naturwissenschaften, Leipzig, Germany

Josef Stoer, Institut für Mathematik, University of Würzburg, Würzburg, Germany

Richard S. Varga, Kent State University, Kent, OH, USA

Harry Yserentant, Institut für Mathematik, Technische Universität Berlin, Berlin, Germany

This is basically a numerical analysis series in which high-level monographs are published. We develop this series aiming at having more publications in it which are closer to applications. There are several volumes in the series which are linked to some mathematical software. This is a list of all titles published in this series.

More information about this series at <http://www.springer.com/series/797>

Kolade M. Owolabi · Abdon Atangana

# Numerical Methods for Fractional Differentiation

 Springer

Kolade M. Owolabi  
Institute for Groundwater Studies  
University of the Free State  
Bloemfontein, South Africa

Abdon Atangana  
Institute for Groundwater Studies  
University of the Free State  
Bloemfontein, South Africa

ISSN 0179-3632                      ISSN 2198-3712 (electronic)  
Springer Series in Computational Mathematics  
ISBN 978-981-15-0097-8              ISBN 978-981-15-0098-5 (eBook)  
<https://doi.org/10.1007/978-981-15-0098-5>

© Springer Nature Singapore Pte Ltd. 2019

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, expressed or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Singapore Pte Ltd. The registered company address is: 152 Beach Road, #21-01/04 Gateway East, Singapore 189721, Singapore

# Preface

Understanding the behaviours of natural occurrences has always been a major concern for mankind. There are many ways to understand and predict nature. On the one hand, understanding nature outside of academic framework, our ancestors and even non-scholars were able to understand and predict the behaviour of natural phenomena through a long-time observation. On the other hand, scholars rely on investigations that comprise observation, construction of models, solutions of models and finally simulation where observed facts are compared with models, and then, the predictions can follow. One of the most used mathematical tools to construct mathematical models is perhaps differential operators. We have two classes, namely local and non-local. The local or classical differential operator is based on the concept of rate of change, and the change is evaluated using two points. Due to the limitations of this concept for modelling real-world problems, the second concept was introduced and called fractional differential operators. They can be further classified into three sub-groups including fractional differential operators with singular and non-local kernel, and this one uses the power law function as kernel. Fractional differential operators with local and singular kernel use exponential decay law as kernel, and finally, fractional differential operators with non-local and non-singular kernel use the generalized Mittag–Leffler function as kernel. These three mathematical tools have been used in many fields of science and technology with great success. However, the solutions of these models are very hard to obtain analytically, and researchers, therefore, rely on numerical methods to provide an approximate solution that could be used for prediction. In the last decades, several numerical methods have been suggested; however, these methods can only be found in research papers. We aim to present in this book the collection of numerical methods related to fractional differential and integral operators and their applications.

Bloemfontein, South Africa

Kolade M. Owolabi  
Abdon Atangana

# Acknowledgements

We must start by acknowledging the Almighty God for giving us the knowledge, wisdom and strength to write this book, and we say thank you Lord. We sincerely appreciate our wives and children for giving us the time and space to do this work. Their ceaseless roles, prayers and support really counts. We wish to express our sincere gratitude and appreciation to certain individuals and organizations who in one way or the other have contributed and helped to make this research work a reality.

We are ineffably grateful to the University of the Free State, Bloemfontein (UFS), in particular the Department of Research and Development, for various financial support received in the course of writing this book. Acknowledgement is also given to the Department of Mathematical Sciences of the Federal University of Technology, Akure, for granting permission to undergo a research study at UFS.

Acknowledgement is given to Atangana Fractional Calculus Research Group here at IGS in UFS and to certain individuals whose names were not mentioned for their assistance and meaningful discussions which made this book a reality.

# Contents

<b>1</b>	<b>Review of Fractional Differentiation</b>	<b>1</b>
1.1	Special Functions	9
1.1.1	The Gamma Function	9
1.1.2	The Beta Function	11
1.1.3	The Complementary Error Function	14
1.1.4	The Mittag–Leffler Function	15
1.1.5	Laplace Transformation and Convolution	18
1.2	Riemann–Liouville Fractional Differentiation	19
1.3	Caputo Fractional Derivative	27
1.4	Classical Fractional Derivatives	30
1.5	Partial Riemann–Liouville Fractional Derivative	33
1.6	Fractional Operators with Variable Order	36
1.7	Tempered Fractional Differentiation	49
1.7.1	Properties of Tempered Fractional Derivative and Integral	54
1.7.2	Laplace Transforms of the Tempered Fractional Calculus	56
1.8	Caputo–Fabrizio Fractional Differentiation	60
1.8.1	Caputo–Fabrizio Fractional Derivative in Caputo Sense	61
1.8.2	The Laplace Transform of the Caputo–Fabrizio Fractional Derivative	62
1.8.3	Fourier Transform of Fractional Gradient, Divergence and Laplacian	62
1.8.4	Caputo–Fabrizio Fractional Derivative in Riemann–Liouville Sense	64
1.9	Stretch Fractional Differentiation	66
1.10	The Atangana–Baleanu Fractional Derivative and Integral	66

1.11	The Riesz Potential and Riesz Fractional Derivatives . . . . .	70
1.11.1	The Atangana–Gómez Fractional Derivative . . . . .	72
	References . . . . .	77
<b>2</b>	<b>Finite Difference Approximations . . . . .</b>	<b>83</b>
2.1	Finite Difference Approximation Schemes . . . . .	84
2.1.1	Taylor Series and Finite Difference Approximation . . . . .	85
2.1.2	Higher Order Finite Difference Approximation . . . . .	87
2.2	Error Analysis . . . . .	89
2.2.1	Illustrative Example . . . . .	92
2.2.2	Order of Accuracy and Consistency . . . . .	94
2.2.3	Matrix Notation . . . . .	97
2.3	Numerical Stability and Convergence Analysis . . . . .	99
2.3.1	Von Neumann (Fourier Series) Stability Analysis . . . . .	99
2.3.2	Matrix Stability Analysis . . . . .	106
2.3.3	Convergence . . . . .	110
2.3.4	Symmetry . . . . .	114
2.4	Numerical Results . . . . .	115
2.5	Finite Difference Approximations Schemes for Fractional Equations . . . . .	116
2.5.1	Matrix Representation of the Finite Difference Schemes . . . . .	120
2.5.2	Convergence Analysis of Fractional Finite Difference Schemes . . . . .	122
2.5.3	Stability Analysis of Fractional Finite Difference Schemes . . . . .	123
2.6	Numerical Approximation of Time-Fractional Sub-diffusion Process with the Second-Order Implicit Difference Method . . . . .	127
2.6.1	Second-Order Implicit Difference Approximation . . . . .	128
	References . . . . .	135
<b>3</b>	<b>Numerical Approximation of Riemann–Liouville Differentiation . . . . .</b>	<b>139</b>
3.1	Numerical Approximation for Time Derivative . . . . .	139
3.2	Numerical Approximation for Space First-Order Derivative . . . . .	142
3.3	Numerical Approximation for Space Second-Order Derivative . . . . .	145
3.4	Crank–Nicholson Scheme for Time-Fractional Differential Equations in Riemann–Liouville Sense . . . . .	147
3.5	A New Definition of Fractional Time Derivative in Riemann–Liouville Sense . . . . .	153
	References . . . . .	160

- 4 Numerical Approximation of Caputo Differentiation** . . . . . 161
  - 4.1 Numerical Approximation for Time Derivative . . . . . 161
  - 4.2 Numerical Approximation for Space First-Order Derivative . . . . . 163
  - 4.3 Numerical Methods for Fractional Evolution Equations . . . . . 165
    - 4.3.1 Fractional Euler and Adams Methods . . . . . 165
    - 4.3.2 The New Fractional Adams–Bashforth Scheme  
with Caputo Derivative . . . . . 166
    - 4.3.3 Existence and Uniqueness of Solutions . . . . . 168
  - References . . . . . 173
- 5 Numerical Approximation of Caputo–Fabrizio Differentiation** . . . . . 175
  - 5.1 Numerical Approximation for the Caputo–Fabrizio Fractional  
Derivative in Caputo Sense . . . . . 175
  - 5.2 Numerical Approximation for Time Derivative . . . . . 180
  - 5.3 Numerical Approximation for Space First-Order Derivative . . . . . 183
  - 5.4 Numerical Approximation for Space Second-Order  
Derivative . . . . . 187
    - 5.4.1 Three-Step Adams–Bashforth Scheme  
with Caputo–Fabrizio Fractional Derivative . . . . . 189
    - 5.4.2 Stability Analysis . . . . . 190
    - 5.4.3 Applications . . . . . 192
  - References . . . . . 194
- 6 Numerical Approximation of Atangana–Baleanu  
Differentiation** . . . . . 195
  - 6.1 Atangana–Baleanu Fractional Derivative in Caputo Sense . . . . . 195
  - 6.2 Uniqueness and Existence of Solution via Chaotic Process . . . . . 198
  - 6.3 Numerical Experiments . . . . . 200
    - 6.3.1 Example 1 . . . . . 201
  - Reference . . . . . 201
- 7 Application to Ordinary Fractional Differential Equations** . . . . . 203
  - 7.1 Numerical Approximation of Fractional Ordinary Differential  
Equation with the Caputo Derivative . . . . . 203
    - 7.1.1 Numerical Schemes and Stability Analysis . . . . . 204
  - 7.2 Modelling the Spread of Viruses in Computer via the Caputo  
Fractional Derivative . . . . . 209
  - 7.3 Modelling the Spread of River Blindness Disease  
with the Caputo Fractional Derivative . . . . . 214
  - 7.4 Modelling of Nonlinear Interpersonal Relationship  
with Time-Fractional Derivative . . . . . 218
  - 7.5 Modelling of El Niño Chaotic Dynamical System  
with the Caputo, Caputo–Fabrizio and Atangana–Baleanu  
Fractional Derivatives . . . . . 222

7.6 A Novel Fractional Model for the Lassa Hemorrhagic Fever . . . . 235

7.7 Modelling of Ebola Hemorrhagic Fever: Fractional Derivative Approach . . . . . 240

References . . . . . 248

**8 Application to Partial Fractional Differential Equation . . . . . 251**

8.1 Space-Fractional Diffusion Equation with New (Atangana–Gomez) Fractional Derivative in Riemann–Liouville Sense . . . . . 251

8.2 Space-Fractional Diffusion Equation with the Riemann–Liouville Derivative . . . . . 255

8.2.1 Fourier Transform Methods . . . . . 256

8.2.2 Finite Difference Methods . . . . . 258

8.2.3 Predictor–Corrector Method of Approximation . . . . . 259

8.2.4 Fourier Spectral Method for Space-Fractional Reaction–Diffusion . . . . . 261

8.3 Application of Caputo–Fabrizio Derivative to Nonlinear Reaction–Diffusion . . . . . 263

8.3.1 Derivation of the Solution via Iterative Method . . . . . 264

8.3.2 Stability Analysis via Fixed Point Theorem . . . . . 264

8.4 Application of Caputo–Fabrizio Derivative to Transmission Line Model with Losses . . . . . 268

8.4.1 Stability Analysis of the Numerical Scheme with the Caputo–Fabrizio Derivative . . . . . 269

8.5 Application of the Caputo–Fabrizio Derivative in Caputo Sense to Time-Fractional Advection–Diffusion Equation . . . . . 272

8.5.1 Stability Anlalysis of the Numerical Method with the Caputo–Fabrizio Derivative for Caputo Type . . . . . 274

8.5.2 Convergence Analysis of the Numerical Scheme with the Caputo–Fabrizio Derivative for Caputo Type . . . . . 276

8.6 Applications of Fractional Derivatives to Diffusion–Advection Equation . . . . . 277

8.6.1 Riemann–Liouville Approach . . . . . 278

8.6.2 Caputo–Fabrizio–Riemann Approach . . . . . 279

8.6.3 Atangana–Baleanu–Riemann Approach . . . . . 280

8.7 Application to Partial Fractional Differential Equation . . . . . 282

8.7.1 The Fisher Equation . . . . . 283

8.7.2 The Gray–Scott Model . . . . . 300

- 8.8 Application of Riesz Fractional Derivative to Schrödinger Equation . . . . . 310
  - 8.8.1 One-Dimensional Fractional-in-Space Schrödinger Equation . . . . . 311
  - 8.8.2 Two-Dimensional Fractional-in-Space Schrödinger Equation . . . . . 312
  - 8.8.3 Numerical Methods of Discretization . . . . . 314
- 8.9 Numerical Experiments . . . . . 318
  - 8.9.1 One-Dimensional Results for Fractional Schrödinger Equation . . . . . 318
  - 8.9.2 Two-Dimensional Results for Fractional Schrödinger Equation . . . . . 319
  - 8.9.3 Three-Dimensional Results for Fractional Schrödinger Equation . . . . . 322
- References . . . . . 324
- Bibliography . . . . . 327

## About the Authors

**Kolade M. Owolabi** is Senior Lecturer at the Department of Mathematical Sciences, Federal University of Technology, Akure, Nigeria. Holding a PhD in Applied (Numerical) Mathematics, he is the author or coauthor of several research papers, and a regular reviewer for several scientific journals. His areas of research interest include numerical methods and scientific computing for the applied problems that arise from interactions between the natural and life sciences and engineering. His research is a well-balanced combination of analytical investigations and numerical experiments using the finite difference technique, spectral method, and exponential time-differencing schemes to address both integer- and non-integer-order ordinary and partial differential equations.

The main objective of his work is to use mathematical theories and methodologies to gain insights into the qualitative behavior of non-linear dynamical systems arising from the mathematical modeling of natural phenomena in the applied sciences and engineering, with an emphasis on the transmission and control dynamics of human diseases of public health interest, as well as addressing mathematical models arising in population biology for ecological patterns and processes.

**Abdon Atangana** is Full Professor at the Faculty of Natural and Agricultural Science, Institute for Groundwater Studies, University of the Free State (UFS), Bloemfontein, South Africa. He obtained his honors and master's degrees in applied mathematics from the Department of Applied Mathematics at the UFS with distinction. He serves as a reviewer for more than 200 accredited international journals, and has been awarded the world champion of peer review in 2016 and in 2017. He also serves on the editorial boards of more than 20 journals of international repute. Professor Atangana's research interests are in the methods and applications of partial and ordinary differential equations, fractional differential equations, perturbation methods, asymptotic methods, iterative methods, and groundwater modeling. He is the founder of fractional calculus with non-local and non-singular kernels, popular in applied mathematics today. Since 2013, he has

published over 225 research articles in several accredited journals of applied mathematics, applied physics, geohydrology, and biomathematics. He is the author of two books, *Fractional Operators with Constant and Variable Order with Application to Geo-hydrology* and *Derivative with a New Parameter: Theory, Methods and Applications*.

# Chapter 1

## Review of Fractional Differentiation



Fractional calculus can be classified as applicable mathematics. The property and theory of this fractional operator is proper object of study in its own right. Scientists and applied mathematicians, in the last decades, found the fractional calculus useful in various fields such as diffusion, elasticity, electrochemistry, rheology, quantitative biology, probability, scattering theory, transport theory and potential theory. However, many mathematicians and scientists are unfamiliar with this topic possibly because they have not been exposed to its applications. Thus, while the theory of fractional calculus has developed, its use has still lagged behind.

Fractional calculus is the field of mathematical analysis which deals with the investigation and applications of derivatives and integrals of arbitrary order. In fact, the field of fractional calculus is almost as old as the traditional calculus proposed independently by Leibniz and Newton [88, 93]. Scholars of engineering, mathematics and sciences often encounter the differential operators in the form  $\frac{d}{dx}$  or  $\frac{d^2}{dx^2}$ , but only a few thought over it if it is mandatory for the differential order to be integer or not. A well-known example is the extension of meaning of real to complex numbers, and another is the extension of meaning of factorials of integers to that of complex numbers. The question could be, 'why not a complex, fractional, rational or irrational number?'

At the onset of differential and integral calculus, a similar question raised by Leibniz in a letter to L'Hopital on the significance of derivative of noninteger (arbitrary) order: *Is it possible to generalize derivatives of integer order with that of arbitrary or noninteger orders?* In curiosity, L'Hopital replied Leibniz with another question: *What if the order is 1/2?* And Leibniz replied in a letter dated 30th September 1695 (a date many authors cite as the birthday of widely called Fractional calculus) that: *'It will result to a paradox, from which one day useful consequences will be drawn'*. So that question posed by Leibniz over 300 year ago has been a subject of debate and active study till date. It is somewhat labelled as **fractional calculus** which typifies the

generalization of both ordinary differentiation and integration to noninteger order. The term fractional is a misnomer, a more accurate term should be ‘noninteger’, since the order itself can be irrational as well, but it is retained following the prevailing use.

Following Leibniz’s and L’Hopital’s first inquisition, the study of fractional calculus was primarily reserved for the best minds in mathematics. As known, a number of physical phenomena are described by fractional derivatives [127]. This is due to the known fact that fractional operators take into account the system evolution, by considering both the global and local characteristics. In addition, experimental results are sometimes contradicted by integer-order calculus and therefore noninteger-order derivatives may be more suitable [116].

Among the great mathematicians that dabbled with fractional calculus and who have provided significant contributions up to the middle of our century, includes L. Euler (1730), P. S. Laplace (1812), J. B. J. Fourier (1822), N. H. Abel (1823–1826), Liouville [67], B. Riemann (1847), H. Holmgren (1865–67), Grünwald [39], Letnikov [62], Laurent [59], P. A. Nekrassov (1888), A. Krug (1890), J. Hadamard (1892), O. Heaviside (1892–1912), S. Pincherle (1902), G. H. Hardy and J. E. Littlewood (1917–1928), Weyl [121], P. Lévy (1923), A. Marchaud (1927), H. T. Davis (1924–1936), A. Zygmund (1935–1945), E. R. Love (1938–1996), A. Erdélyi (1939–1965), H. Kober (1940), D. V. Widder (1941), Riesz [105]. Afterwards, fractional calculus has become an attractive subject to engineers, mathematicians and physicists, and various forms of noninteger (that is, fractional) differential operators such as the Grünwald–Letnikov, Hadamard, Riemann–Liouville, Caputo, Riesz (Hilfer [44], Kilbas et al. [52], Podlubny [101], Samko et al. [110], Cresson [26], Katugampola [50], Kilbas and Saigo [51] and Klimek [54, 55]) were introduced. Agrawal [4] introduced an interesting perspective to the subject by unifying all previously mentioned notions of fractional derivatives and integrals, and later studied in Bourdin et al. [14].

Many found, using their own notation and methodology, definitions that are well fitted to the concept of an arbitrary (noninteger) order derivative or integral. The most famous of these definitions that have been widely popularized in the world of fractional calculus are the Riemann–Liouville, Grünwald–Letnikov and Caputo definitions. In what follows, we briefly consider some of the initial and notable definitions of fractional calculus.

- L. Euler (1730):  
Euler generalized the formula

$$\frac{d^r x^q}{dx^r} = q(q-1) \cdots (q-r+1)x^{q-r}$$

with the aid of the gamma function

$$\Gamma(q+1) = q(q-1) \cdots (q-r+1)\Gamma(q-r+1)$$

to get

$$\frac{d^r x^q}{dx^r} = \frac{\Gamma(q + 1)}{\Gamma(q - r + 1)} x^{q-r}.$$

The gamma function is defined as

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt, \quad \text{Re}(z) > 0.$$

- J. B. J. Fourier (1820–1822):  
By using integral representation

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^\infty f(z) dz \int_{-\infty}^\infty \cos(\nu x - \nu z) d\nu$$

Fourier wrote

$$\frac{d^r f(x)}{dx^r} = \frac{1}{2\pi} \int_{-\infty}^\infty f(z) dz \int_{-\infty}^\infty \cos(\nu x - \nu z + \frac{r\pi}{2}) d\nu.$$

- N. H. Abel (1823–1826):  
Abel considered the integral

$$\int_0^x \frac{p'(\xi) d\xi}{(x - \xi)^\alpha} = \psi(x)$$

for arbitrary  $\alpha$  and then writes

$$p(x) = \frac{1}{\Gamma(1 - \alpha)} \frac{d^{-\alpha} \psi(x)}{dx^{-\alpha}}.$$

- J. Liouville (1832–1855):  
The first definition was based on exponential representation of a function  $f(x) = \sum_{r=0}^\infty c_r e^{a_r x}$ , he generalized the formula  $\frac{d^q e^{ax}}{dx^q} = a^q e^{ax}$  as

$$\frac{d^s f(x)}{dx^s} = \sum_{r=0}^\infty c_r a_r^s e^{a_r x}.$$

The second definition was fractional integral

$$\int^\mu \Psi(x) dx^\mu = \frac{1}{(-1)^\mu \Gamma(\mu)} \int_0^\infty \Psi(x + \alpha) \alpha^{\mu-1} d\alpha$$

$$\int^\mu \Psi(x) dx^\mu = \frac{1}{\Gamma(\mu)} \int_0^\infty \Psi(x - \alpha) \alpha^{\mu-1} d\alpha.$$

By using  $\tau = x + \alpha$  and  $\tau = x - \alpha$ , respectively, in above formulas, he got

$$\int^{\mu} \Psi(x) dx^{\mu} = \frac{1}{(-1)^{\mu} \Gamma(\mu)} \int_x^{\infty} (\tau - x)^{\mu-1} \Psi(\tau) d\tau$$

$$\int^{\mu} \Psi(x) dx^{\mu} = \frac{1}{\Gamma(\mu)} \int_{-\infty}^x (\tau - x)^{\mu-1} \Psi(\tau) d\tau.$$

The third definition involves fractional derivative

$$\frac{d^{\mu} f(x)}{dx^{\mu}} = \frac{(-1)^{\mu}}{h^{\mu}} \left( f(x) \frac{\mu}{1!} f(x+h) + \frac{\mu(\mu-1)}{2!} f(x+2h) - \dots \right)$$

$$\frac{d^{\mu} f(x)}{dx^{\mu}} = \frac{1}{h^{\mu}} \left( f(x) \frac{\mu}{1!} f(x-h) + \frac{\mu(\mu-1)}{2!} f(x-2h) - \dots \right).$$

- G. F. B. Riemann (1847–1876):  
He defines fractional integral as

$$D^{-s} f(x) = \frac{1}{\Gamma(s)} \int_c^x (x-t)^{s-1} f(t) dt + \phi(t).$$

- N. Ya. Sonin (1869), A.V. Letnikov (1872), H. Laurent (1884), N. Nekrasove (1888), K. Nishimoto (1987–):  
They considered the Cauchy integral formula

$$f^{(r)}(z) = \frac{r!}{2\pi i} \int_c \frac{f(t)}{(t-z)^{r+1}} dt$$

which when replaced  $r$  by  $s$ , yields

$$d^s f(z) = \frac{\Gamma(s+1)}{2\pi i} \int_c^{x^+} \frac{f(t)}{(t-z)^{s+1}} dt.$$

- Riemann–Liouville:  
This is one of mostly celebrated definition of fractional calculus which combines the two previous definitions.

$${}_a D_t^{\alpha} f(t) = \frac{1}{\Gamma(r-\alpha)} \left( \frac{d}{dt} \right)^r \int_a^t \frac{f(\tau)}{(t-\tau)^{\alpha-r+1}} d\tau.$$

- Grünwald–Letnikov:  
The combined definition is given as

$${}_a D_t^{\alpha} f(t) = \lim_{h \rightarrow 0} h^{-\alpha} \sum_{j=0}^{\left[ \frac{t-a}{h} \right]} (-1)^j \binom{\alpha}{j} f(t-jh).$$

- M. Caputo (1967):  
The second most popular definition is given by

$${}^C D_t^\alpha f(t) = \frac{1}{\Gamma(\alpha - n)} \int_a^t \frac{f^{(n)}(\tau)}{(t - \tau)^{\alpha+1-n}} d\tau, \quad (n - 1 \leq \alpha < n).$$

- K. S. Miller, B. Ross (1993):  
They used differential operator  $D$  as

$$D^{\bar{\alpha}} f(t) = D^{\alpha_1} D^{\alpha_2} \dots D^{\alpha_n} f(t), \quad \bar{\alpha}(\alpha_1, \alpha_2, \dots, \alpha_n),$$

where  $D^{\alpha_i}$ ,  $i = 1, 2, \dots, n$  is Riemann–Liouville or Caputo definitions.

Fractional calculus has since mentioned from the inception of classical calculus, but it was not until 1823 before fractional operations were first utilized to address a specific physical problem. Though Euler and Fourier made mention of derivatives of arbitrary order, they neither gave applications nor reporting any example. As a result, the honour of giving the first application was credited to Niels Henrik Abel [1, 2]. Abel applied the fractional calculus to solve an integral equation which arises in the formulation of the tautochrone problem

$$k = \int_0^x (x - t)^{-1/2} f(t) dt, \tag{1.0.1}$$

where  $f$  is an unknown function to be determined. This problem, which is commonly referred to as the isochrone problem, it has to do with finding the shape of a frictionless wire in a vertical plane such that the time of slide of a bead placed on the wire slides to the lowest point of the wire in the same time regardless of where the bead is placed. The brachistochrone problem deals with the shortest time of slide.

In the classical book by Samko et al. [110], they opined that it is important to note that Abel not only solved the integral equation (1.0.1) as the special case of the tautochrone problem, but he provided the solution for the integral equation in a more general form

$$k(x) = \int_a^x \frac{f(t)}{(x - t)^\alpha} dt, \quad x > a, \quad 0 < \alpha < 1. \tag{1.0.2}$$

Years after Abel’s application of fractional operators to a problem in physics, series of broad papers were written by Liouville on fractional calculus [70, 72]. In article [71], Liouville comes up with two different definitions of fractional derivatives. The first definition is applied on functions  $f(x)$  which can be expanded in a series form

$$f(x) = \sum_{k=0}^{\infty} c_k \exp(a_k x).$$

By applying the known classical order derivatives  $d^n/dx^n \exp(ax) = D^n e^{ax} = a^n e^{ax}$  to the fractional type (replacing  $n \in \mathbb{N}$  with  $\alpha \in \mathbb{C}$ ), he got

$$D^\alpha f(x) = \sum_{k=0}^{\infty} c_k a_k^\alpha \exp(a_k x). \quad (1.0.3)$$

Obviously, the first definition is somewhat restricted owing to the choices of fractional index  $\alpha$  for which series (1.0.3) is converged. There is no such restriction on the choice of  $\alpha$  in the second definition reported in [71], but rather faced a more stronger restriction based on the type of function for which it is applied. For a function with an arbitrary parameter  $a$  of the case  $f(x) = 1/x^a$ , Liouville developed the definition

$$D^\alpha x^{-a} = \frac{(-1)^\alpha \Gamma(a + \alpha)}{\Gamma(a)} x^{-a-\alpha} \quad (1.0.4)$$

to be its fractional derivative of order  $\alpha$ . Despite the fact that both definitions given in [71] were somehow restricted, Liouville still applied these definitions in a number of applications to physical, geometrical and mechanical problems. A number of theoretical and applied results can be found in the Liouville eight papers [70, 72].

In 1847, Riemann worked on a research paper where he searched for the generalization of a Taylor series and came up with the definition

$$D^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_c^x (x-t)^{\alpha-1} f(t) dt + \phi(x) \quad (1.0.5)$$

for a given function  $f(x)$  with fractional integral order  $\alpha$ . The function  $\phi(x)$  is introduced as a result of the ambiguity of the lower limit  $c$  of integration which corresponds to the complementary function as reported in the Liouville work. Equation (1.0.5) with lower limit  $c = 0$  and without a complementary function  $\phi(x)$  is the most widely celebrated definition of fractional integration today, known as the Riemann–Liouville fractional integral.

Since neither Riemann nor Liouville addressed the problem of the complementary function, it is now of historical interest how the Riemann–Liouville definition was finally developed. A quite number of researchers are actually responsible for this development: In 1869, Sonin [112] wrote a paper, where he adopted Cauchy's Integral formula as a starting point to reach differentiation with arbitrary index. A short time later in 1872, Letnikov extended the idea of Sonin in his paper [64].

Both attempted to define fractional derivatives by using a closed contour. Beginning with Cauchy's integral formula for integer-order derivatives, defined by

$$f^{(n)}(z) = \frac{n!}{2\pi i} \int_c \frac{f(t)}{(t-z)^{n+1}} dt, \quad (1.0.6)$$

which by replacing the factorial with Euler's gamma function  $\alpha! = \Gamma(\alpha + 1)$ , one obtains the generalization to the fractional case. In [60], Laurent introduced an open

circuit contour as against a closed circuit used by both Sonin and Letnikov which lead to the popular Riemann–Liouville fractional integral

$${}_c D_x^{-\alpha} f(x) = \frac{1}{\Gamma(\alpha)} \int_c^x (x - t)^{\alpha-1} f(t) dt, \quad \text{Re}(\alpha) > 0 \quad (1.0.7)$$

by standard contour integration techniques. By letting  $c = 0$  in (1.0.7) one obtains the Riemann formula (1.0.5) without the issues of complementary function  $\phi(x)$  problem, and by setting  $c = -\infty$ , formula (1.0.7) becomes the first Liouville definition (1.0.3). These two findings substantiate why the above formula is referred to as the Riemann–Liouville fractional integral equation. The notation of fractional differentiation and integration differs only in sign of the fractional-order  $\alpha$ , changing from fractional differentiation to integration or vice versa cannot be achieved directly if one replaces the sign of parameter  $\alpha$  on the right-hand side of formula (1.0.7). The problematic issue originates from the integral  $\int_c^x (x - t)^{-\alpha-1} f(t) dt$  which in general case diverged. Though by analytic continuation it can be proved that

$${}_c D_x^\alpha f(x) = {}_c D_x^{n-\beta} f(x) = {}_c D_x^n {}_c D_x^{-\beta} f(x) = \frac{d^n}{dx^n} \left( \frac{1}{\Gamma(\beta)} \int_c^x (x - t)^{\beta-1} f(t) dt \right) \quad (1.0.8)$$

is satisfied, which is globally referred to as the definition of the Riemann–Liouville fractional derivative.

Almost at the same time with Sonin paper [112], to start with the mathematical basis for nowadays version of the Riemann–Liouville fractional integral, two historic papers, the first by Grünwald [40] and the other by Letnikov [63] have given the basis for another definition of fractional derivative which is often used till today. As definition for fractional differentiation, Grünwald and Letnikov obtained

$${}^{GL} D_x^\alpha f(x) = \lim_{h \rightarrow 0} \frac{(\Delta_h^\alpha f)(x)}{h^\alpha} \quad (1.0.9)$$

which is known as Grünwald–Letnikov fractional derivative. In (1.0.9), the finite differences  $\Delta_h^\alpha$  are defined as

$$(\Delta_h^\alpha f)(x) = \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} f(x - kh), \quad \alpha > 0,$$

where  $\binom{\alpha}{k}$  is known as the generalized binomial coefficient. Today, the Grünwald–Letnikov definition of fractional derivatives is used for numerical methods, which applies formula (1.0.9) in conjunction with a finite sum for the approximation of fractional derivatives.

The Riemann–Liouville definition of a fractional integral defined in (1.0.7) with  $c = -\infty$  is commonly called Weyl fractional integral. Check the work of Weyl [122]

that was published in 1917 where he considered the Fourier transform of periodic functions  $\phi(x)$  as

$$\sum_{k=-\infty}^{\infty} \phi_k e^{ikx}, \quad \text{for } \phi_k = \frac{1}{2\pi} \int_0^{2\pi} e^{ikx} \phi(x) dx$$

in attempt to define fractional integration that is suitable for these functions, by

$$I_{\pm}^{\alpha} \phi(x) = \frac{1}{2\pi} \int_0^{2\pi} \Xi_{\pm}^{\alpha}(x-t) \phi(t) dt,$$

where  $\Xi_{\pm}^{\alpha}(x)$  are some special functions. In addition, he showed that these fractional integrals can be written in the interval  $0 < \alpha < 1$  as

$$I_{+}^{\alpha} \phi(x) = \frac{1}{\Gamma(\alpha)} \int_{-\infty}^x (x-t)^{\alpha-1} \phi(t) dt \quad \text{and} \quad I_{-}^{\alpha} \phi(x) = \frac{1}{\Gamma(\alpha)} \int_x^{\infty} (x-t)^{\alpha-1} \phi(t) dt \quad (1.0.10)$$

which are convergent over an infinite interval. This convergence is guaranteed in Weyl's paper by considering only those periodic functions  $\phi(x)$ , whose Fourier transform is shown to have fulfilled  $\phi_0 = 0$ . Weyl showed in [122] that a periodic continuous function  $\phi(x)$  has a continuous derivative of order  $\alpha$  if it satisfies a Lipschitz condition of order  $\alpha$ .

Integral version of Grünwald–Letnikov definition of fractional derivative was developed by Marchaud [82] in 1927, using

$${}^M D^{\alpha} f(x) = c \int_0^{\infty} \frac{(\Delta_t^{\ell} f)(x)}{t^{1+\alpha}} dt, \quad \text{for } \alpha > 0, \quad (1.0.11)$$

as fractional derivative of function  $f$ , where  $c$  is regarded as a normalizing constant and the term  $(\Delta_t^{\ell} f)(x)$  is a finite difference of order  $\ell > \alpha$ . Marchaud introduces a new definition for noninteger order of derivatives. This definition coincides with the Liouville version for sufficiently good functions [27, 77]. Equation (1.0.11) is referred to as Marchaud fractional derivative. Under certain conditions, the above definition coincides with both Grünwald–Letnikov and Riemann–Liouville version of fractional derivatives.

Wantanabe [120] in 1931 developed a version of Leibniz formula for Riemann–Liouville fractional derivative, defined by

$$D^{\alpha}(fg) = \sum_{k=-\infty}^{\infty} \binom{\alpha}{k+\beta} D^{\alpha-\beta-k} f D^{\beta+k} g, \quad \beta \in \mathbb{R} \quad (1.0.12)$$

for analytic functions  $f$  and  $g$ .

Years later, Riesz began to publish a number of research articles that are centred around the integral [106, 107]

$${}^R I^\alpha \phi = \frac{1}{2\Gamma(\alpha) \cos(\alpha\pi/2)} \int_{-\infty}^{\infty} \frac{\phi(t)}{|t-x|^{1-\alpha}} dt, \quad \text{Re } \alpha > 0, \quad \alpha \neq 1, 3, 5, \dots \quad (1.0.13)$$

known as Riesz potential. The above integral is tightly connected with both Weyl fractional integral and the Riemann–Liouville fractional integrals by

$${}^R I^\alpha = (I_+^\alpha + I_-^\alpha) (2 \cos(\alpha\pi/2))^{-1}.$$

In [31, 32], Erdélyi and Kober introduced a modification to the definition of the Riemann–Liouville fractional integral as

$$\frac{2x^{2(\alpha+\xi)}}{\Gamma(\alpha)} \int_0^x (x^2-t)^{\alpha-1} t^{2\xi+1} \phi(t) dt, \quad \frac{2x^{2\xi}}{\Gamma(\alpha)} \int_0^\infty (x^2-t)^{\alpha-1} t^{1-2\alpha-2\xi} \phi(t) dt$$

which are found useful in almost application areas today. A good number of additional results of fractional calculus were reported in the twentieth century, here we shall consider in addition the one presented by Caputo [18]. Given a function  $f$  with  $(n-1)$  as a continuous derivative, Caputo defined his own version of a fractional derivative as

$$D_*^\alpha f(x) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-s)^{n-\alpha-1} \left(\frac{d}{ds}\right)^n f(s) ds \quad (1.0.14)$$

which is labelled today as the Caputo fractional derivative.

## 1.1 Special Functions

Understanding of definitions and use of fractional calculus will be made more simple and clearer by taking a tour of some necessary but relatively simple mathematical definitions that will evolve in the study of these concepts. These include the gamma function, the beta function, the Laplace transform, and the Mittag–Leffler function and the complementary error function are briefly addressed in this section. Many others are classified in Guo [41], Samko et al. [110] and Podlubny [101] to mention a few.

### 1.1.1 The Gamma Function

The gamma function  $\Gamma(z)$  is considered as a generalization of the factorial notation  $q!$  for all real numbers, that is,  $\Gamma(q) = (q-1)!$  for  $q \in \mathbb{N}$ . Assume  $z$  is a complex number with positive real number (that is,  $\text{Re } z > 0$ ), then the integral

$$\Gamma(z) = \int_0^{\infty} e^{-t} t^{z-1} dt$$

which converges absolutely is called the gamma function, or simply the Euler integral equation of the second kind. It is clear from the known result that  $\Gamma(1) = 1$ . By adopting integration by parts technique, we have

$$\int_0^{\infty} e^{-t} t^z dt = -e^{-t} t^z \Big|_{t=0}^{t=\infty} + z \int_0^{\infty} e^{-t} t^{z-1} dt,$$

which lead to a basic property of the gamma function

$$\Gamma(z + 1) = z\Gamma(z), \quad (1.1.1)$$

also when  $z \in \mathbb{N}^+$ ,  $\Gamma(z) = (z - 1)!$ . The beauty of the gamma function is inherent in its properties. As seen in (1.1.1), this function is known to be unique in that the value for any quantity is, by virtue of the form of the integral which is equivalent to that quantity  $z$  minus one times the gamma of the quantity minus one.

By using this property, we generalize the gamma function into the type  $\mathbf{Re}z < 0$ . When  $-p < \mathbf{Re}z \leq -p + 1$ , we define

$$\Gamma(z) = \frac{\Gamma(z + p)}{z(z + 1) \cdots (z + p - 1)}.$$

**Proposition 1.1.1** *There satisfies the Euler's reflection formula*

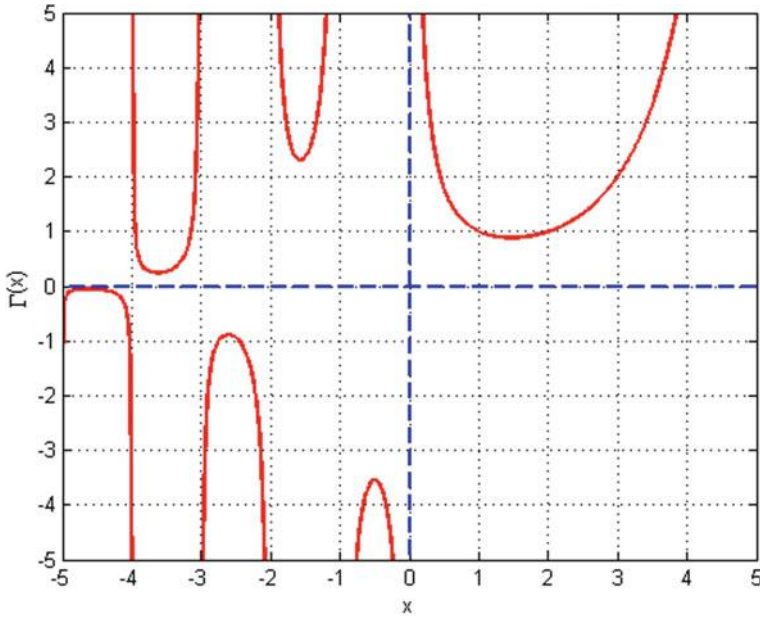
$$\Gamma(z)\Gamma(1 - z) = \frac{\pi}{\sin(\pi z)}$$

for any  $z$  with  $\mathbf{Re}z \notin \mathbf{Z}$ .

The function is extended to the whole complex plane by analytic continuation except for the points  $0, -1, -2, \dots$ , with simple poles, see [101] for details. Thus  $\Gamma : \mathbb{C} \setminus \{0, -1, -2, \dots\} \rightarrow \mathbb{C}$ . The graph of the gamma function is displayed in Fig. 1.1

Some of the basic properties are summarized below:

$$\begin{aligned} \Gamma(1) &= 1, \\ \Gamma(z + 1) &= z\Gamma(z), \\ \Gamma(q) &= (q - 1)!, \quad q \in \mathbb{N}, \\ \Gamma(q + 1) &= q!, \quad \forall q \in \mathbb{N}, \\ \Gamma(1/2) &= \sqrt{\pi}, \\ \Gamma(q + 1/2) &= \frac{\sqrt{\pi}}{2^q} (2q - 1)!!, \quad q \in \mathbb{N}. \end{aligned}$$



**Fig. 1.1** Approximation of Gamma function for real argument

A full list of well-known properties of the gamma function can be found in Gradshteyn and Ryzhik [37].

### 1.1.2 The Beta Function

The beta is also referred to as the Euler integral equation of the first kind, the beta function has an important relationship in the study of fractional calculus. Its solution can be defined through the use of multiple gamma function, as well share a form that is characteristically similar to fractional derivative or integral several functions, in particular, the polynomials of the form  $t^a$  and the Mittag–Leffler function.

The beta function, denoted as  $\beta(z, w)$ , is defined by

$$\beta(z, w) = \int_0^1 (1 - u)^{z-1} u^{w-1} du = \frac{(w - 1)!(z - 1)!}{(w + z - 1)!} = \beta(w, z), \quad z, w \in \mathbb{R}^+ \tag{1.1.2}$$

conventionally denoted as

$$\beta(z, w) = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z + w)}, \quad \mathbf{Re}z > 0, \mathbf{Re}w > 0.$$

Equation (1.1.2) demonstrates the beta integral and its solution in terms of the gamma function.

To derive the integral representation of the beta function, we require to express the product of two factorial as

$$p!q! = \int_0^\infty e^{-u} u^p du \int_0^\infty e^{-v} v^q dv.$$

Let  $u = x^2$  and  $v = y^2$ , so that

$$p!q! = 4 \int_0^\infty e^{-u^2} x^{2p+1} dx \int_0^\infty e^{-v^2} y^{2q+1} dy = \int_{-\infty}^\infty \int_{-\infty}^\infty e^{-(x^2+y^2)} |x|^{2p+1} |y|^{2q+1} dx dy$$

to transform to polar coordinates, we substitute with  $x = r \cos \theta$  and  $y = r \sin \theta$ , so that

$$p!q! = \int_0^{2\pi} \int_0^\infty e^{-v^2} |r \cos \theta|^{2p+1} |r \sin \theta|^{2q+1} r dr d\theta$$

to obtain

$$p!q! = 2(p+q+1)! \int_0^{\frac{\pi}{2}} \cos^{2p+1} \theta \sin^{2q+1} \theta d\theta$$

the beta function is then defined by

$$\beta(p+1, q+1) = 2 \int_0^{\frac{\pi}{2}} \cos^{2m+1} \theta \sin^{2n+1} \theta d\theta = \frac{p!q!}{(p+q+1)!}.$$

By rewriting the arguments, we obtain the usual form for the beta function

$$\beta(w, z) = \frac{\Gamma(w)\Gamma(z)}{\Gamma(w+z-1)}.$$

The beta function arises from the gamma function

$$\beta(z, w) = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)} = \frac{(z-1)!(w-1)!}{z+w-1},$$

where  $\Gamma$  typifies the gamma function. We can derive the relationship between the beta and the gamma functions as

$$\Gamma(x)\Gamma(y) = \int_0^\infty e^{-u} u^{x-1} du \int_0^\infty e^{-v} v^{y-1} dv.$$

Next, we let  $u = a^2$  and  $v = b^2$  so that

$$\Gamma(x)\Gamma(y) = 4 \int_0^\infty e^{-b^2} b^{2y+1} db \int_0^\infty e^{-a^2} a^{2x+1} da = \int_{-\infty}^\infty \int_{-\infty}^\infty e^{-(a^2+b^2)} |a|^{2x-1} |b|^{2y-1} dadb.$$

To transform into polar coordinates we make use of substitutions  $a = r \cos \theta$  and  $b = r \sin \theta$ , so that

$$\begin{aligned} \Gamma(x)\Gamma(y) &= \int_0^{2\pi} \int_0^\infty e^{-r^2} |r \cos \theta|^{2x-1} |r \sin \theta|^{2y-1} r dr d\theta \\ &= \int_0^\infty e^{-r^2} r^{2x+2y-2} r dr \int_0^{2\pi} |(\cos \theta)^{2x-1} (\sin \theta)^{2y-1}| d\theta \\ &= \Gamma(x+y)\beta(x, y). \end{aligned}$$

Again, we rewrite the arguments with the usual form of beta function to obtain

$$\beta(z, w) = \frac{\Gamma(z)\Gamma(w)}{\Gamma(z+w)}. \tag{1.1.3}$$

**Lemma 1.1.2** *The gamma function satisfies for the Legendre formula*

$$\Gamma(z)\Gamma\left(z + \frac{1}{2}\right) = \sqrt{\pi} 2^{1-2z} \Gamma(2z).$$

*Proof* Let  $\text{Re } z > 0$ , so that

$$\beta(z, z) = \int_0^1 (t(1-t))^{z-1} dt.$$

Assume  $\xi = 4t(1-t)$ , then

$$\beta(z, z) = 2 \int_0^{1/2} (t(1-t))^{z-1} dt = \frac{1}{2^{2z-1}} \int_0^1 \xi^{z-1} (1-\xi)^{-1/2} d\xi = 2^{1-2z} \beta(z, 1/2)$$

leading to the Legendre formula.

Considering the beta function, the standard binomial coefficient

$$C_q^s = \frac{q!}{s!(q-s)!} = \frac{\Gamma(1+q)}{\Gamma(1+s)\Gamma(1+q-s)}$$

which we generalize into

$$C_{-\varrho}^\varsigma = \frac{\Gamma(1-\varrho)}{\Gamma(1+\varsigma)\Gamma(1-\varrho-\varsigma)},$$

where  $\varrho$  and  $\varsigma$  are regarded as complex numbers. If  $\varsigma = s$ , a positive integer, then Proposition 1.1.1 simply implies

$$C_{-\varrho}^s = \frac{\Gamma(1-\varrho)}{s!\Gamma(1-\varrho-s)} = (-1)^s \frac{\Gamma(s-\varrho)}{s!\Gamma(\varrho)} = (-1)^s C_{\varrho+s-1}^s.$$

□

*Remark 1.1.3* It should be noted that Eq. (1.1.3) gives the analytical continuation of the beta function in the entire complex plane through the analytical continuation of the gamma function.

**Proposition 1.1.4** *The beta function is symmetric, if*

$$\beta(z, w) = \beta(w, z).$$

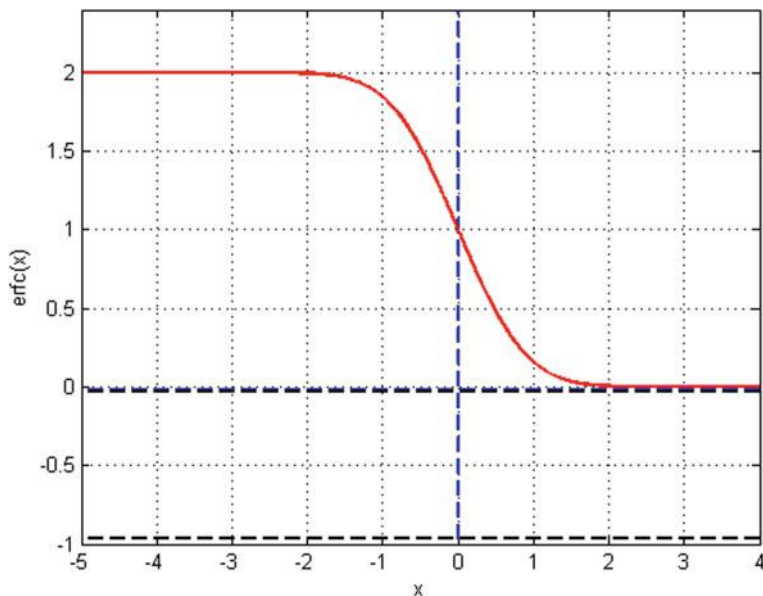
*Proof* The proof of Proposition 1.1.4 follows directly from definition (1.1.2).  $\square$

### 1.1.3 The Complementary Error Function

The complementary error function is an entire function, defined by

$$\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt. \quad (1.1.4)$$

The graph of (1.1.4) is displayed in Fig. 1.2.



**Fig. 1.2** The complementary error function

Special values of the complementary error function include

$$\begin{aligned}\operatorname{erfc}(-\infty) &= 2, \\ \operatorname{erfc}(0) &= 1, \\ \operatorname{erfc}(+\infty) &= 0.\end{aligned}$$

The following useful relations should be noted:

$$\begin{aligned}\operatorname{erfc}(-x) &= 2 - \operatorname{erfc}(x), \\ \int_0^\infty \operatorname{erfc}(x) dx &= \frac{1}{\sqrt{\pi}}, \\ \int_0^\infty \operatorname{erfc}^2(x) dx &= \frac{2 - \sqrt{2}}{\sqrt{\pi}}.\end{aligned}$$

### 1.1.4 The Mittag–Leffler Function

The Mittag–Leffler function naturally occurs in the solution of fractional differential equations or fractional-order integral equations, and particularly in the investigations of the fractional generalization of the Lévy flights, random walk, kinetic equation, superdiffusive processes and in the study of complex and spatiotemporal dynamical systems. The generalized and ordinary Mittag–Leffler functions interpolate between a power law and exponential-law behaviour of phenomena controlled by ordinary kinetic equations and their fractional counterparts, see, for example, [44, 56–58].

The fractional derivative operator offers a means of distinguishing between a homogeneous and simple system that exhibits local, Gaussian behaviour, and one that is heterogeneous and relatively complex, with non-local, power-law behaviour [47, 78, 84, 94, 123, 124]. However, attempt to compute and solve a fractional partial differential equation often results in a difficult task, which require efficient and reliable numerical methods that are able to tackle the dynamics [49, 99, 100]. In addition, the closed-form solution to a fractional partial differential equation, particularly in the situation where the fractional time derivative, appears in the form of a convergent power series of the Mittag–Leffler case, which requires considerable computational burden for efficient, reliable and accurate calculation [45, 79]. The Mittag–Leffler function has been applied across many disciplines, for instance: anomalous diffusion applications [30, 47, 87], biochemical transport kinetics [48], molecular transport [36], information processing in neural networks [23, 125], viscoelasticity in polymer networks [38, 119], heat conduction [102], scaling behaviour in human travel [15] and signal processing [95] among many others.

The Mittag–Leffler function is a generalization of the exponential function, while the gamma function is a generalization of the factorial function [101]. The Mittag–Leffler function is defined as a power series expansion

$$f(z) = E_\alpha(z) = \sum_{s=0}^{\infty} \frac{z^s}{\Gamma(\alpha s + 1)}, \quad \alpha > 0, \quad \alpha \in \mathbb{R}, \quad z \in \mathbb{C}, \quad (1.1.5)$$

where  $E_\alpha$  is the single-parameter Mittag–Leffler function [89], and  $\Gamma$  is the generalized form of factorial function, valid for real numbers [43]. When  $\alpha = 1$ , through the property  $\Gamma(s + 1) = s!$ , then Eq. (1.1.5) becomes

$$f(z) = E_1(z) = \sum_{s=0}^{\infty} \frac{z^s}{s!}, \quad (1.1.6)$$

which is known as the Taylor series definition of the exponential function.

The two-parameter generalization of the Mittag–Leffler function which plays an important role in the fractional calculus was first introduced by Agarwal [3], is defined by the series expansion

$$E_{\alpha,\beta}(z) = \sum_{s=0}^{\infty} \frac{z^s}{\Gamma(\alpha s + \beta)}, \quad \alpha > 0, \quad \beta > 0 \quad \alpha, \beta \in \mathbb{R}, \quad z \in \mathbb{C}. \quad (1.1.7)$$

When  $\beta = 1$  in (1.1.7), we denote  $E_\alpha(z) = E_{\alpha,1}(z)$  to be a one-parameter Mittag–Leffler function. When both  $\alpha, \beta$  are real and positive, above series converge for values of  $z$  and the Mittag–Leffler function is an entire function. Approximation of the Mittag–Leffler function for different values of  $\alpha$  and  $\beta$  is displayed in Fig. 1.3.

Some important properties of the Mittag–Leffler functions are [101]:

$$\begin{aligned} E_{1,1}(z) &= e^z, \\ E_{2,1}(z^2) &= \cosh(z), \quad E_{1,2}(z) = \frac{e^z - 1}{z}, \\ E_{2,2}(z^2) &= \frac{\sinh(z)}{z}, \quad E_{2,2}(z) = \frac{\sinh(z)}{\sqrt{z}}, \\ E_{\alpha,1}(z) &= E_\alpha(z), \\ E_{1/2,1}(z) &= e^{z^2} \operatorname{erfc}(-z), \end{aligned}$$

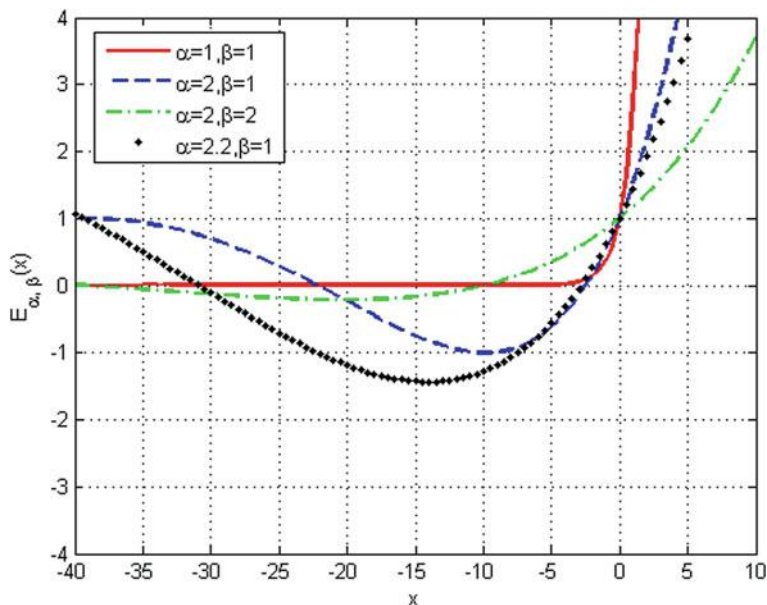
where  $\operatorname{erfc}(z)$  is termed the complementary error function. Other special cases of the Mittag–Leffler function  $E_\alpha(z)$  include

$$E_0(z) = \frac{1}{1 - z}, \quad |z| < 1,$$

$$E_1(z) = e^z,$$

$$E_2(z) = \cosh(\sqrt{z}), \quad z \in \mathbb{C},$$

$$E_2(-z^2) = \cos z, \quad z \in \mathbb{C},$$



**Fig. 1.3** Approximation of two-parameter Mittag–Leffler function at different instances of  $\alpha$  and  $\beta$

$$E_3(z) = \frac{1}{2} \left[ e^{z^{1/3}} + 2e^{-(1/2)z^{1/3}} \cos \left( \frac{\sqrt{3}}{2} z^{1/3} \right) \right], \quad z \in \mathbb{C},$$

$$E_4(z) = \frac{1}{2} [\cos(z^{1/4}) + \cosh(z^{1/4})], \quad z \in \mathbb{C},$$

$$E_{1/2}(\pm z^{1/2}) = e^z [1 + \operatorname{erf}(\pm z^{1/2})] = e^z \operatorname{erfc}(\pm z^{1/2}), \quad z \in \mathbb{C},$$

where  $\operatorname{erfc}(z)$  remains the complementary error function and the error function  $\operatorname{erf}(z)$  is defined as

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-t^2) dt, \quad \operatorname{erfc}(z) = 1 - \operatorname{erf}(z), \quad z \in \mathbb{C}.$$

The case of half-integer ( $q/2$ ) can be written as

$$E_{q/2}(z) = {}_0F_{q-1} \left( \begin{matrix} \frac{1}{q}, \frac{2}{q}, \dots, \frac{q-1}{q}, \frac{z^2}{q^q} \end{matrix} ; \frac{2^{(q+1)/2} z}{q! \sqrt{\pi}} \right) {}_1F_{2q-1} \left( \begin{matrix} 1; \frac{q+2}{2q}, \frac{q+3}{2q}, \dots, \frac{3q}{2q}; \frac{z^2}{q^q} \end{matrix} \right).$$

The generalized multi-index Mittag–Leffler function is defined by means of the power series in Kiryakova [53] as

$$E_{(1/\phi_i),(\varphi_i)}(z) = \sum_{s=0}^{\infty} \psi_s z^s = \sum_{s=0}^{\infty} \frac{z^s}{\prod_{j=1}^p \Gamma(\varphi_j + s/\phi_j)},$$

where  $m > 1$  is an integer,  $\phi_1, \dots, \phi_p$  and  $\varphi_1, \dots, \varphi_p$  are arbitrary but real parameters.

### 1.1.5 Laplace Transformation and Convolution

The Laplace transform is a function transformation that is used to solve most complicated differential equations. With the Laplace transform, it is often possible to circumvent working with equations of different differential order directly by translating the equation into a domain where the solution presents itself algebraically. The usual definition of the Laplace transform is defined as

$$\mathcal{L}\{f(t)\} = \int_0^{\infty} e^{-st} f(t) dt = \bar{f}(s). \quad (1.1.8)$$

If Eq. (1.1.8) is a convergent integral, then we say that the Laplace transform of the function  $f(t)$  exists. The basic criteria for this is that function  $f(t)$  must not grow at the rate higher than that at which the exponential term  $e^{-st}$  is decreasing.

The Laplace convolution is given by

$$f(t) * g(t) = \int_0^t f(t - \tau)g(\tau)d\tau = g(t) * f(t). \quad (1.1.9)$$

It should be mentioned that the convolution of two functions in the domain of  $t$  is somewhat complicated to solve, however, the convolution leads to simple function multiplication in the Laplace domain, that is,

$$\mathcal{L}\{f(t) * g(t)\} = \bar{f}(s)\bar{g}(s).$$

The Laplace transform of a derivative of integer order  $q$  of the function  $f(t)$ , is defined by

$$\mathcal{L}\{f^{(q)}(t)\} = s^q \bar{f}(s) - \sum_{j=0}^{q-1} s^{q-j-1} f^{(j)}(0) = s^q \bar{f}(s) - \sum_{j=0}^{q-1} s^q f^{(q-j-1)}(0).$$

The Laplace transforms for some known Mittag–Leffler function are given in a summarized form (Magin [78], Podlubny [101])

$$\begin{aligned}\mathcal{L}\{E_\alpha(-\lambda t^\alpha)\} &= \frac{s^{\alpha-1}}{s^\alpha + \lambda}, & \mathcal{L}\{t^{\alpha-1}E_{\alpha,\alpha}(-\lambda t^\alpha)\} &= \frac{1}{s^\alpha + \lambda}, \\ \mathcal{L}\{t^{\beta-1}E_{\alpha,\beta}(-\lambda t^\alpha)\} &= \frac{s^{\alpha-\beta}}{s^\alpha + \beta}, & \mathcal{L}\{\mathcal{E}_k(t, \pm\lambda; \alpha, \beta)\} &= \frac{k!s^{\alpha-\beta}}{(s^\alpha \pm \lambda)^{k+1}}.\end{aligned}\tag{1.1.10}$$

## 1.2 Riemann–Liouville Fractional Differentiation

Riemann's modified version of Liouville's fractional integral operator is a direct generalization of Cauchy's formula for an  $n$ -fold integral [110]

$$\int_a^x dx_1 \int_a^{x_1} dx_2 \cdots \int_a^{x_{n-1}} f(x_n) dx_n = \frac{1}{(n-1)!} \int_a^x \frac{f(t)}{(x-t)^{1-n}} dt, \tag{1.2.1}$$

knowing that  $(n-1)! = \Gamma(n)$ , Riemann realized that the right-hand side of (1.2.1) could have meaning if  $n$  takes noninteger values. Thus, fractional integration is defined as follows.

**Definition 1.2.1** If  $f(x) \in C([a, b])$  and  $a < x < b$ , then

$$I_{a+}^\alpha f(x) := \frac{1}{\Gamma(\alpha)} \int_a^x \frac{f(t)}{(x-t)^{1-\alpha}} dt$$

where  $\alpha \in (-\infty, \infty)$  is known as the Riemann–Liouville fractional integral of order  $\alpha$ . Similarly, for  $\alpha \in (0, 1)$  we have

$$D_{a+}^\alpha f(x) := \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x \frac{f(t)}{(x-t)^\alpha} dt \tag{1.2.2}$$

which is labelled as the Riemann–Liouville fractional derivative of order  $\alpha$ .

These operators are commonly addressed as the Riemann–Liouville fractional integral operators. The special fractional derivative scenario is when  $\alpha = 1/2$ , called the semi-derivative. The connection between the fractional derivative and integral based on what Riemann realized can be dated back to the solvability of Abel's integral formula for the interval  $\alpha \in (0, 1)$  as

$$f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x \frac{\phi(t)}{(x-t)^{1-\alpha}} dt, \quad \text{for } x > 0. \tag{1.2.3}$$

By changing  $x$  to  $t$  and  $t$  to  $s$ , respectively, Eq. (1.2.3) can further be solved by multiplying its both sides by  $(x-t)^{-\alpha}$  and then integrate to obtain

$$\int_a^x \frac{dt}{(x-t)^\alpha} \int_a^t \frac{\varphi(s) ds}{(t-s)^{1-\alpha}} = \Gamma(\alpha) \int_a^x \frac{f(t) dt}{(x-t)^\alpha}.$$

By applying Fubini's theorem to interchange the order of integration in the left-hand side we get

$$\int_a^x \varphi(s) ds \int_s^x \frac{dt}{(x-t)^\alpha (t-s)^{1-\alpha}} = \Gamma(\alpha) \int_a^x \frac{f(t) dt}{(x-t)^\alpha}.$$

With change of variable  $t = s + \tau(x-s)$  and adopt the beta function formula, one can easily evaluate the inner integral as

$$\int_a^x (x-t)^{-\alpha} (t-s)^{\alpha-1} dt = \int_0^1 \tau^{\alpha-1} (1-\tau)^{-\alpha} d\tau = B(\alpha, 1-\alpha) = \Gamma(\alpha)\Gamma(1-\alpha).$$

Hence, we obtain

$$\int_a^x \varphi(s) ds = \frac{1}{\Gamma(1-\alpha)} \int_a^x \frac{f(t) dt}{(x-t)^\alpha}.$$

By differentiating, we get

$$\varphi(x) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_a^x \frac{f(t) dt}{(x-t)^\alpha}. \quad (1.2.4)$$

Therefore, if Eq. (1.2.3) has a solution that is given by (1.2.4) which satisfies  $\alpha \in (0, 1)$ . Obviously, one can deduce that (1.2.3) is the  $\alpha$ -order integral while the inversion (1.2.4) is the  $\alpha$ -order derivative.

An important fact concerning the Riemann–Liouville operators is that the following semi-group property of fractional integrals is satisfied.

**Theorem 1.2.2** For any function  $f \in C([a, b])$ , the Riemann–Liouville integral

$$I_{a+}^\alpha I_{a+}^\beta f(x) = I_{a+}^{\alpha+\beta} f(x)$$

holds for  $\alpha > 0, \beta > 0$ .

*Proof* By definition, we have

$$I_{a+}^\alpha I_{a+}^\beta f(x) = \frac{1}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x \frac{dt}{(x-t)^{1-\alpha}} \int_a^t \frac{f(u)}{(t-u)^{1-\beta}} du,$$

since  $f(x) \in C([a, b])$ , we can set  $t = u + s(x-u)$  and applying Fubini's theorem, we get

$$I_{a+}^\alpha I_{a+}^\beta f(x) = \frac{B(\alpha, \beta)}{\Gamma(\alpha)\Gamma(\beta)} \int_a^x \frac{f(u)}{(x-t)^{1-\alpha-\beta}} du = I_{a+}^{\alpha+\beta} f(x).$$

□

In what follows, we extend the Riemann–Liouville to hold for a larger set of  $\alpha$ , we let  $\alpha = \bar{\alpha} + \hat{\alpha}$ , where  $\bar{\alpha}$  stands for the integer part of  $\alpha$ , and  $\hat{\alpha}$  represents the remainder part.

**Definition 1.2.3** If  $\alpha > 0$  is not an integer, then we define

$$D_{a+}^{\alpha} f = \frac{d^{\bar{\alpha}}}{dx^{\hat{\alpha}}} D_{a+}^{\hat{\alpha}} f = \frac{d^{\bar{\alpha}+1}}{dx^{\hat{\alpha}+1}} I_{a+}^{1-\hat{\alpha}} f,$$

thus

$$D_{a+}^{\alpha} f(x) = \int_1^{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x \frac{f(t) dt}{(x-t)^{\alpha-n+1}},$$

for any  $f \in C^{\bar{\alpha}+1}([a, b])$  if  $n = \bar{\alpha} + 1$ . If otherwise, that is  $\alpha < 0$  then the notation

$$D_{a+}^{\alpha} f = I_{a+}^{-\alpha} f$$

may be regarded as the definition.

Obviously, for  $\alpha < 0$  there exists the fractional derivative  $D_{a+}^{\alpha} f(x)$  for all  $f \in C([a, b])$  and for all  $x \in [a, b]$ . We also remark that for  $\alpha > 0$ , certainly there exists the fractional derivative  $D_{a+}^{\alpha} f(x)$  for all  $f \in C^{\bar{\alpha}+1}([a, b])$  and all  $x \in (a, b)$ . To expatiate on this, we write  $n = \bar{\alpha} + 1$  and apply the Taylor's formula

$$f(t) = \sum_{k=0}^{n-1} \frac{f^{(k)}(a)}{k!} (t-a)^k + \frac{1}{(n-1)!} \int_a^t \frac{f^{(n)}(s)}{(t-s)^{n-1}} ds, \quad \forall t \in [a, b].$$

On putting the above into the definition of  $D_{a+}^{\alpha} f(x)$  and simplify the integral we get

$$\begin{aligned} D_{a+}^{\alpha} f(x) &= \frac{d^n}{dx^n} \left( \sum_{k=0}^{n-1} \frac{f^{(k)}(a)}{\Gamma(k+2-\hat{\alpha})} (x-a)^{k+1-\hat{\alpha}} \right. \\ &\quad \left. + \frac{1}{\Gamma(n+1-\hat{\alpha})} \int_a^x f^{(n)}(s) \cdot (x-s)^{n-\hat{\alpha}} ds \right). \end{aligned} \quad (1.2.5)$$

Obviously, the above derivative is valid for all  $x \in (a, ]$ , the integral becomes resolvable since  $f^{(n)} \in C([a, b])$  bear in mind that the exponent  $n - \hat{\alpha}$  is larger than  $n - 1$ , so that  $\frac{d^k}{dx^k} (x-s)^{n-\hat{\alpha}}$  is integrable for all  $k = 0, 1, 2, \dots, n$ . This justifies our assertion.

**Definition 1.2.4** For  $\alpha > 0$ , let  $I_{a+}^{\alpha}$  be the space functions which can be denoted by the Riemann–Liouville integral order  $\alpha$  for some  $C([a, b])$ -function.

This definition leads to the following theorem.

**Theorem 1.2.5** Let  $f \in C([a, b])$  and  $\alpha > 0$ . In order that  $f(x) \in I_{a+}^{\alpha}([a, b])$ , it becomes necessary and sufficient that

$$I_{a+}^{n-\alpha} f \in C^n([a, b]), \quad (1.2.6)$$

where  $n = \bar{\alpha} + 1$ , and that

$$\left( \frac{d^k}{dx^k} I_{a+}^{n-\alpha} f(x) \right)_{x=a} = 0, \quad k = 0, 1, 2, \dots, n-1. \quad (1.2.7)$$

*Proof* Let  $f(x) \in I_{a+}^\alpha([a, b])$ , then  $f(x) = I_{a+}^\alpha g(x)$  for some  $g \in C([a, b])$ . By Theorem 1.2.2, we obtain

$$\begin{aligned} I_{a+}^{n-\alpha} f(x) &= I_{a+}^{n-\alpha} I_{a+}^\alpha g(x) = I_{a+}^n g(x) = \frac{1}{(n-1)!} \int_a^x \frac{g(t)}{(x-t)^{1-n}} dt \\ &= \int_a^x dx_1 \int_a^{x_1} dx_2 \cdots \int_a^{x_{n-1}} g(x_n) dx_n. \end{aligned}$$

This shows that (1.2.6) satisfies, and by repeated differentiation, it is obvious that Eq. (1.2.7) also holds.

In converse, if we assume that  $f \in C([a, b])$  holds (1.2.6) and (1.2.7). By applying Taylor's formula to function  $I_{a+}^{n-\alpha} f$ , we get

$$I_{a+}^{n-\alpha} f(t) = \int_a^t \frac{d^n}{ds^n} I_{a+}^{n-\alpha} f(s) \cdot \frac{(t-s)^{n-1}}{(n-1)!} ds \quad \forall t \in [a, b].$$

If we write  $\phi(t) = \frac{d^n}{ds^n} I_{a+}^{n-\alpha} f(s)$ , bear in mind that  $\phi \in C([a, b])$  in (1.2.6). And, by semi-group property in Theorem 1.2.2 and Definition 1.2.1, above relation shows that

$$I_{a+}^{n-\alpha} f(t) = I_{a+}^n \phi(t) = I_{a+}^{n-\alpha} I_{a+}^\alpha \phi(t),$$

and thus

$$I_{a+}^{n-\alpha} (f - I_{a+}^\alpha \phi) \equiv 0.$$

By following a general fact about uniqueness of any solution to Abel's integral equation (see, Samko et al. Lemma 2.5 [110]), bear in mind that  $n - \alpha$  is positive, this shows that  $f \equiv I_{a+}^\alpha \phi$ , and thus  $f \in I_{a+}^\alpha([a, b])$ .  $\square$

**Theorem 1.2.6** *If  $\alpha > 0$  then the equality*

$$D_{a+}^\alpha I_{a+}^\alpha f = f(x) \quad (1.2.8)$$

*is satisfied for any  $f \in C([a, b])$ . Now let  $f \in C^{\bar{\alpha}+1}([a, b])$ , then for the equality*

$$I_{a+}^\alpha D_{a+}^\alpha f(x) = f(x) \quad (1.2.9)$$

*to satisfy we assume that  $f$  holds for the condition in Theorem 1.2.5, otherwise*

$$I_{a+}^\alpha D_{a+}^\alpha f(x) = f(x) - \sum_{k=0}^{n-1} \frac{(x-a)^{\alpha-k-1}}{\Gamma(\alpha-k)} \frac{d^{n-k-1}}{dx^{n-k-1}} (I_{a+}^{n-\alpha} f(x)) \quad (1.2.10)$$

*satisfies.*

*Proof* By definition, we have

$$D_{a+}^{\alpha} I_{a+}^{\alpha} f = \frac{1}{\Gamma(\alpha)\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x \frac{dt}{(x-t)^{\alpha-n+1}} \int_a^t \frac{f(s)ds}{(t-s)^{1-\alpha}}. \quad (1.2.11)$$

By employing the Fubini's theorem, interchange the order of integration and evaluate the inner integral to obtain

$$D_{a+}^{\alpha} I_{a+}^{\alpha} f = \frac{1}{\Gamma(n)} \frac{d^n}{dx^n} \int_a^x \frac{f(s)}{(x-s)^{n-1}} ds, \quad (1.2.12)$$

then Eq. (1.2.8) follows from (1.2.12) by Cauchy's formula (1.2.1). again, since  $f$  in (1.2.9) holds for the conditions in Theorem 1.2.5 and  $f \in C^{\bar{\alpha}+1}([a, b])$  it directly follows by (1.2.7) that Eq. (1.2.8) is satisfied. On the other hand, let us assume that the function  $f \in C^{\bar{\alpha}+1}([a, b])$  does not hold for condition in (1.2.7) as given in Theorem 1.2.5. This implies that the residue outside the integration will not vanish as in (1.2.8) but as integration is deployed, one obtains (1.2.10) by induction.  $\square$

An interesting property of the Riemann–Liouville operators prior to investigations on non-differentiability and its relation to fractional calculus is that certain non-differentiable functions such as Weierstrass and Riemann functions seem to have fractional derivative of all orders in the interval  $(0, 1)$  [33]. This contributes to the problem that the relation between the fractional and ordinary derivatives is not entirely obvious, but a clearer picture on some of their correlation might be given by the following theorem.

**Theorem 1.2.7** *If  $f \in C^1([a, b])$ ,  $f(a) \geq 0$  and  $\alpha \in (0, 1)$ , then  $D_{a+}^{\alpha} f(x)$  is non-negative if  $f$  is increasing on  $[a, x]$ .*

*Proof* Since  $f \in C^1([a, b])$  one can employ (1.2.5) and let  $n = \bar{\alpha} + 1 = 1$  which leads to

$$D_{a+}^{\alpha} f(x) = \frac{f(a)}{\Gamma(1-\alpha)} (x-a)^{-\alpha} + \frac{1}{\Gamma(1-\alpha)} \int_a^x f'(s) (x-s)^{-\alpha} ds. \quad (1.2.13)$$

Since  $\Gamma(1-\alpha) > 0$  for all  $0, \alpha < 1$  and  $x > 0$ , knowing well that  $f(a) \geq 0$ . We can say the first right-hand term in (1.2.13) is nonnegative. Now, we are left show that the second right-hand term that contains the integral is nonnegative too. Knowing that  $f'(s) \geq 0$  on  $[a, x]$  since  $f$  is an increasing function. More so  $(x-s)^{-\alpha} > 0$  for  $s \in [a, x]$  which shows that the integral is nonnegative. The proof is completed.  $\square$

For fractional calculus in the complex plane, as a direct generalization of the Riemann–Liouville fractional derivative and integral for the analytic functions we have the following definitions.

**Definition 1.2.8** For any analytic function  $f$  on some open simply connected domain which contains the points  $z$  and  $z_0$ , we define for any  $\alpha > 0$

$$I_{z_0}^\alpha f(z) = \frac{1}{\Gamma(\alpha)} \int_{z_0}^z \frac{f(t)}{(z-t)^{1-\alpha}} dt, \quad (1.2.14)$$

$$D_{z_0}^\alpha f(z) = \frac{d^q}{dz^q} I_{z_0}^{q-\alpha} f(z), \quad q = \bar{\alpha} + 1, \quad (1.2.15)$$

along the line connecting two points  $z$  and  $z_0$ . We refer to (1.2.14) as the fractional integral of analytic function  $f(z)$  of order  $\alpha$ . The definition  $D_{z_0}^\alpha f = I_{z_0}^{-\alpha} f$  for  $\alpha < 0$  shall be used.

We select the principal value for  $(z-t)^{1-\alpha}$ , and fix the point  $z$  to interpret the integral equation (1.2.14) uniquely. We let

$$0 \leq \arg(z-z_0) < 2\pi, \quad (1.2.16)$$

in attempt to coincide with  $\arg(z-t) = \arg(z-z_0)$ . Thus, we get

$$(z-t)^{1-\alpha} = |z-t|^{1-\alpha} e^{i(1-\alpha)\arg(z-z_0)}, \quad (1.2.17)$$

thus (1.2.14) is defined uniquely. Also, the semi-group property of fractional integral in Theorem 1.2.2 satisfies for (1.2.14) for any  $\alpha > 0$ ,  $\beta > 0$ , its proof is similar to that of Theorem 2 in [110]. Fractional differentiation in addition to complex fractional integral by using contour integration in the complex plane become a valuable and frequently used tool in fractional calculus [61, 110]. We give equivalent Cauchy integral formula

$$D^n F(z) = \frac{n!}{2\pi i} \oint \frac{F(t)}{(t-z)^{n+1}} dt$$

for arbitrary nonnegative integral values of  $n$ .

**Theorem 1.2.9** Let  $f(z) = (z-z_0)^\varrho \xi(z)$ , for  $\varrho > -1$  and  $\xi(z)$  is analytic in simply connected domain  $\Xi$  that contains the points  $z$  and  $z_0$ , subject to principal value (1.2.16) of  $(z-z_0)^\varrho$ . The Cauchy fractional derivative of order  $\alpha$

$$D_{z-z_0}^\alpha F(z) = \frac{\Gamma(\alpha+1)}{2\pi i} \int_{C(z_0, z^+)} F(t)(t-z)^{-\alpha-1} dt \quad (1.2.18)$$

of  $f$  equivalent to the complex generalization of Riemann–Liouville fractional-order derivative

$$D_{z-z_0}^\alpha f(z) = D_{z_0}^\alpha f(z)$$

for all  $\alpha \in \mathbb{R}$ , except for  $\alpha \in \mathbb{Z}$ .

*Proof* We start with  $\alpha < 0$  (for  $\alpha \neq -1, -2, \dots$ ). Known that the integrand of (1.2.18) is analytic in  $\Xi$  we deform  $C(z_0, z^+)$  into contours  $C_1, C_2$  and  $C_3$ , where  $C_1$  denotes the line segment from  $z_0$  to  $z$ ,  $C_2$  represents the circle centred at point  $t = z$  and  $C_3$  is the transverse of  $C_1$  in the opposite direction. By adopting the Cauchy integral theorem, we obtain

$$\begin{aligned} D_{z-z_0} f(z) &= \frac{\Gamma(1+\alpha)}{2\pi} \int_{C(z_0, z^+)} f(t)(t-z)^{-1-\alpha} dt \\ &= \frac{\Gamma(1+\alpha)}{2\pi} \left( \int_{C_1} \dots dt + \int_{C_2} \dots dt + \int_{C_3} \dots dt \right). \end{aligned} \quad (1.2.19)$$

□

By the jump  $(t-z)^{-1-\alpha}$  at the cut, we obtain

$$\begin{aligned} \frac{\Gamma(1+\alpha)}{2\pi} \int_{C(z_0, z^+)} \frac{f(t)}{(t-z)^{1+\alpha}} dt &= \frac{\Gamma(1+\alpha)}{2\pi} (1 - e^{2\alpha\pi i}) \int_{z_0}^z \frac{f(t)}{(t-z)^{1+\alpha}} dt \\ &\quad + \frac{\Gamma(1+\alpha)}{2\pi} \lim_{\delta \rightarrow 0} \delta^{-\alpha} \int_0^{2\pi} f(z + \delta e^{i\varphi}) e^{-i\alpha\varphi} d\varphi. \end{aligned} \quad (1.2.20)$$

Clearly, with condition (1.2.16) and precise choices  $-\pi \leq \arg(t-z) < \pi$  and  $\pi \leq \arg(t-z) < 3\pi$  at the start and end points of  $C(z_0, z^+)$ , respectively, it is noticeable that  $(t-z)^{-1-\alpha} = e^{(1+\alpha)\pi i} (z-t)^{-1-\alpha}$  which coincides with the values in (1.2.17) when we replaced  $1-\alpha$  by  $-1-\alpha$ . Since  $((s^{i\pi\alpha} - e^{-i\pi\alpha})/2i)\Gamma(\alpha+1) = \sin(\pi\alpha)\Gamma(\alpha+1) = -\pi/\Gamma(-\alpha)$ , by (1.2.20), we have

$$\frac{\Gamma(1+\alpha)}{2\pi} \int_{C(z_0, z^+)} \frac{f(t)}{(t-z)^{1+\alpha}} dt = I_{z_0}^{-\alpha} f(z) \quad (1.2.21)$$

It is obvious that Eq. (1.2.18) is the same as (1.2.14) for  $\alpha < 0$  except when  $\alpha = -1, -2, -3, \dots$ . For  $\alpha > 0$ , we utilize the complex derivative (1.2.15) after replacing  $\alpha$  with  $\alpha - \hat{\alpha} - 1$  and differentiating (1.2.21) to get (1.2.18). This is satisfied since the contour of integration require only to be perturbed slightly for the start and end points to be at  $z_0$ , thus we only require to differentiate the integrand with respect to  $z$  when deploying  $d^n/dz^n$ . This also satisfies for  $\alpha \neq 0, 1, 2, \dots$ , thus the proof is completed.

A more complex result for the classical case was defined by Leibniz' formula as generalized product rule. For Riemann–Liouville derivatives, a similar result can be obtained.

**Theorem 1.2.10** (Leibniz' formula for Riemann–Liouville fractional derivative) *Let  $\alpha > 0$  and assume that both functions  $f$  and  $g$  are analytic on the open interval  $(a-h, a+h)$ . Then,*

$$D_a^\alpha [fg] = \sum_{n=0}^{[\alpha]} \binom{\alpha}{n} (D^n f)(x) (D_a^{\alpha-n} g)(x) + \sum_{n=[\alpha]+1}^{\infty} \binom{\alpha}{n} (D^n f)(x) (\mathbf{J}_a^{n-\alpha} g)(x)$$

for  $a < x < a + h/2$ .

*Proof* Before we prove Theorem 1.2.10, let us consider the following corollaries.

**Corollary 1.2.11** *Let function  $f$  be analytic in  $(a-h, a+h)$  for some  $h > 0$ , and let  $\alpha > 0$ ,  $\alpha \notin \mathbb{N}$ . Then*

$$D_a^\alpha f(x) = \sum_{n=0}^{\infty} \binom{\alpha}{n} \frac{(x-a)^{n-\alpha}}{\Gamma(n+1-\alpha)} D^n f(x)$$

for  $a < x < a + h/2$ , and

$$D_a^\alpha f(x) = \sum_{n=0}^{\infty} \frac{(x-a)^{n-\alpha}}{\Gamma(n+1-\alpha)} D^n f(x)$$

for  $a < x < a + h$  and  $D_a^\alpha$  is analytic in  $(a, a + h)$ .

**Corollary 1.2.12**

$$\mathbf{J}_a^\alpha f(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (x-a)^{n+\alpha}}{n!(\alpha+n)\Gamma(\alpha)} D^n f(x)$$

for  $a < x < a + h/2$ , and

$$\mathbf{J}_a^\alpha f(x) = \sum_{n=0}^{\infty} \frac{(x-a)^{n+\alpha}}{\Gamma(n+1+\alpha)} D^n f(x)$$

for  $a < x < a + h$  and  $\mathbf{J}_a^\alpha$  is analytic in  $(a, a + h)$ .

With respect to Corollary 1.2.11, we obtain

$$D_a^\alpha [fg](x) = \sum_{n=0}^{\infty} \binom{\alpha}{n} \frac{(x-a)^{n-\alpha}}{\Gamma(n+1-\alpha)} D^n [fg](x).$$

By applying the standard Leibniz formula to operator  $D^n [fg]$  and interchange the order of summation, gives

$$\begin{aligned}
D_a^\alpha [fg](x) &= \sum_{n=0}^{\infty} \binom{\alpha}{n} \frac{(x-a)^{n-\alpha}}{\Gamma(n+1-\alpha)} \sum_{i=0}^n \binom{\alpha}{i} D^i f(x) D^{n-i} g(x) \\
&= \sum_{i=0}^{\infty} \sum_{n=0}^{\infty} \binom{\alpha}{n} \frac{(x-a)^{n-\alpha}}{\Gamma(n+1-\alpha)} \binom{n}{i} D^i f(x) D^{n-i} g(x) \\
&= \sum_{i=0}^{\infty} D^i f(x) \sum_{\sigma=0}^{\infty} \binom{\alpha}{\sigma+i} \frac{(x-a)^{\sigma+i-\alpha}}{\Gamma(\sigma+i+1-\alpha)} \binom{\sigma+i}{i} D^\sigma g(x).
\end{aligned}$$

The observation  $\binom{\alpha}{\sigma+i} \binom{\sigma+i}{i} = \binom{\alpha}{i} \binom{\alpha-i}{\sigma}$  yields

$$\begin{aligned}
D_a^\alpha [fg](x) &= \sum_{i=0}^{\infty} D^i f(x) \binom{\alpha}{i} \sum_{\sigma=0}^{\infty} \binom{\alpha-i}{\sigma} \frac{(x-a)^{\sigma+i-\alpha}}{\Gamma(\sigma+i+1-\alpha)} D^\sigma g(x) \\
&= \sum_{i=0}^{[\alpha]} \binom{\alpha}{i} D^i f(x) \sum_{\sigma=0}^{\infty} \binom{\alpha-i}{\sigma} \frac{(x-a)^{\sigma+i-\alpha}}{\Gamma(\sigma+i+1-\alpha)} D^\sigma g(x) \\
&\quad + \sum_{i=[\alpha]+1}^{\infty} \binom{\alpha}{i} D^i f(x) \sum_{\sigma=0}^{\infty} \binom{\alpha-i}{\sigma} \frac{(x-a)^{\sigma+i-\alpha}}{\Gamma(\sigma+i+1-\alpha)} D^\sigma g(x).
\end{aligned}$$

The desired result follows by considering the first parts of Corollaries 1.2.11 and 1.2.12, then replace the inner sums.  $\square$

### 1.3 Caputo Fractional Derivative

Caputo fractional derivative is seen as a good alternative method to the Riemann–Liouville type for computing fractional derivative. It was first introduced in the research work [18] by M. Caputo and two years later in his book [19]. The Caputo fractional derivative of order  $\alpha$ -th for a function  $f$  can be written as

$${}_a^C D_t^\alpha = \frac{1}{\Gamma(q-\alpha)} \int_a^t \frac{f^{(q)}(\xi)}{(t-\xi)^{\alpha+1-\xi}} d\xi, \quad (q-1 < \alpha < q). \quad (1.3.1)$$

The Caputo fractional derivative here is denoted by  ${}_a^C D_t^\alpha$  to distinguish it from the Riemann–Liouville fractional derivative. Under natural and normal conditions on  $f$ , when  $a = 0$ , the Caputo fractional derivative of  $\alpha$ -th order can be simplified as  ${}^C D^\alpha$ . Also, we observed that when  $\alpha \rightarrow q$  the Caputo fractional derivative reduces to a classical  $q$ -th derivative of the function  $f(t)$  [41, 101]. Assuming that  $0 \leq q-1 < \alpha < q$  and that the function  $f(t)$  is continuously bounded derivatives on closed interval  $[a, T]$ , for every  $T > a$ . Then

$$\begin{aligned} \lim_{\alpha \rightarrow q} {}^C D_t^\alpha f(t) &= \lim_{\alpha \rightarrow q} \left( \frac{f^{(q)}(a)(t-a)^{q-\alpha}}{\Gamma(q-\alpha+1)} + \frac{1}{\Gamma(q-\alpha+1)} \int_a^t (t-\xi)^{q-\alpha} f^{(q+1)}(\xi) d\xi \right) \\ &= f^{(q)}(a) + \int_a^t f^{(q+1)}(\xi) d\xi = f^{(q)}(t), \quad q = 1, 2, \dots \end{aligned}$$

By definition and integration by parts, we obtain

$${}^C D^\alpha f(t) = \frac{f^{(q)}(0)t^{q-\alpha}}{\Gamma(q-\alpha+1)} + \int_0^t \frac{(t-\xi)^{q-\alpha} f^{(q+1)}(\xi)}{\Gamma(q-\alpha+1)} d\xi.$$

This indicates that the Caputo technique also provides an interpolation between the integer-order derivatives, similar to the Riemann–Liouville and the Grünwald–Letnikov approaches. The main advantage of Caputo’s technique is that the initial conditions for fractional differential equation with the Caputo derivatives take on the same form as for classical order differential equations.

The order of differentiation is the major difference between the Riemann–Liouville and Caputo fractional derivatives. In the Caputo fractional derivative, it first takes the integer-order classical derivative and then the fractional-order derivative. But the reverse is the case for the Riemann–Liouville derivative. In addition, the Caputo fractional derivative of a constant (say,  $c$ ) is zero, while it is not zero for the case of the Riemann–Liouville fractional derivative at the lower terminal  $a$ , but

$${}_0 D_t^\alpha c = \frac{ct^{-\alpha}}{\Gamma(1-\alpha)}.$$

Next, we want to make comparison between the Riemann–Liouville and Caputo fractional derivatives, this can be achieved by expressing both in the form of the Riemann–Liouville fractional integrals. The  $\gamma$ -th order Riemann–Liouville fractional integral can be defined as

$$D^{-\gamma} f(t) = \frac{1}{\Gamma(\gamma)} \int_0^t \frac{f(\xi)}{(t-\xi)^{1-\gamma}}, \quad \gamma > 0.$$

The Riemann–Liouville fractional derivative can be written in terms of the Riemann–Liouville fractional integral  $D^{-\gamma}$  as

$${}^{RL} D_t^\alpha f(t) = \frac{1}{\Gamma(\gamma)} \frac{d^\gamma}{dt^\gamma} \int_0^t \frac{f(\xi) d\xi}{(t-\xi)^{1-\gamma}} = \frac{d^\gamma}{dt^\gamma} [D^{-\gamma} f(t)],$$

for  $\gamma = q - \alpha > 0$ . In the same way for  $\gamma = q - \alpha > 0$ , the Caputo fractional derivative can be defined as

$${}^C D_t^\alpha f(t) = \frac{1}{\Gamma(\gamma)} \int_0^t \frac{f(\xi) d\xi}{(t-\xi)^{1-\gamma}} = D^{-\gamma} \left[ \frac{d^\gamma}{dt^\gamma} f(t) \right].$$

These two derivatives are related by

$${}^{RL}D_t^\alpha f(t) = {}^C D_t^\alpha f(t) + \sum_{n=0}^{q-1} \frac{t^{n-\alpha}}{\Gamma(n-\alpha+1)} f^{(n)}(0),$$

for  $t > 0$  on the semi closed interval  $q - 1 < \alpha \leq p$ . The right-hand side of the above equation is equivalent to the Grünwald–Letnikov definition of fractional derivative, which requires that  $f(t)$  be  $q$  times continuously differentiable on  $\alpha \in (q - 1, q]$ . But the Riemann–Liouville definition provides a better opportunity to weaken the conditions on  $f(t)$ . Since the Riemann–Liouville fractional derivative weakens the condition  $f(t)$ , this encourages many scholar to widely adapt the Caputo fractional derivative to initial value problems arising from differential equations with strong physical interpretations.

We would also like to present another clear difference between the Caputo and the Riemann–Liouville approaches, which has been mentioned in [101], that it is of important interest for applications. For the Caputo derivative, we get

$${}^C D_t^\alpha ({}^C D_t^p f(t)) = {}^C D_t^{\alpha+p} f(t), \text{ for } p = 0, 1, 2, \dots, \quad q - 1 < \alpha < p$$

while for the case of Riemann–Liouville derivative, we have

$${}_a \mathbf{D}_t^p ({}_a \mathbf{D}_t^\alpha f(t)) = {}_a \mathbf{D}_t^{\alpha+p} f(t), \text{ for } p = 0, 1, 2, \dots, \quad q - 1 < \alpha < p.$$

The following conditions are found satisfied when the differential operators in the last two equations are interchanged:

$$\begin{aligned} {}^C D_t^\alpha ({}^C D_t^p f(t)) &= {}^C D_t^p ({}^C D_t^\alpha f(t)) = {}^C D_t^{\alpha+p} f(t), \\ f^{(x)}(0) &= 0, \quad x = q, q + 1, \dots, p, \text{ for } p = 0, 1, 2, \dots; \quad q - 1 < \alpha < q \end{aligned}$$

and

$$\begin{aligned} {}_a \mathbf{D}_t^p ({}_a \mathbf{D}_t^\alpha f(t)) &= {}_a \mathbf{D}_t^\alpha ({}_a \mathbf{D}_t^p f(t)) = {}_a \mathbf{D}_t^{\alpha+p} f(t), \\ f^{(x)}(0) &= 0, \quad x = 0, 1, 2, \dots, p \text{ for } p = 0, 1, 2, \dots; \quad q - 1 < \alpha < q. \end{aligned}$$

It is obvious here that the Caputo fractional derivative has no restriction on the values  $f^{(x)}(0)$ ,  $x = 0, 1, \dots, q - 1$ .

**Theorem 1.3.1** (Leibniz' formula for Caputo fractional derivatives) *Let  $0 < \alpha < 1$ , and assume that both functions  $f$  and  $g$  are analytic on the interval  $(a - h, a + h)$ . Then,*

$${}^C D_a^\alpha [fg](x) = \frac{(x-a)^{-\alpha}}{\Gamma(1-\alpha)} g(a)[f(x) - f(a)] + (D_a^\alpha g(x)) f(x) + \sum_{n=1}^{\infty} \binom{\alpha}{n} (\mathbf{J}_a^{n-\alpha} g(x)) D_a^n f(x).$$

*Proof* By applying the definition of the Caputo fractional operator, we have

$${}^c D_{\mathbf{a}}^\alpha [fg] = D_{\mathbf{a}}^\alpha [fg - f(a)g(a)] = D_{\mathbf{a}}^\alpha [fg] - f(a)g(a)D_{\mathbf{a}}^\alpha [1].$$

In what follows, we apply Leibniz formula for the Riemann–Liouville fractional derivatives and obtain

$$D_{\mathbf{a}}^\alpha [fg] = f(D_{\mathbf{a}}^\alpha g) + \sum_{n=1}^{\infty} \binom{\alpha}{n} (D_{\mathbf{a}}^n f) (\mathbf{J}_{\mathbf{a}}^{n-\alpha} g) - f(a)g(a)D_{\mathbf{a}}^\alpha [1].$$

On adding and subtracting  $f(a)g(a)(D_{\mathbf{a}}^\alpha [1])$  and rearrange, we get

$$\begin{aligned} D_{\mathbf{a}}^\alpha [fg] &= f(D_{\mathbf{a}}^\alpha [g - g(a)]) + \sum_{n=1}^{\infty} \binom{\alpha}{n} (D_{\mathbf{a}}^n f) (\mathbf{J}_{\mathbf{a}}^{n-\alpha} g) + g(a)(f - f(a))D_{\mathbf{a}}^\alpha [1] \\ &= f(D_{\mathbf{a}}^\alpha g) + \sum_{n=1}^{\infty} \binom{\alpha}{n} (D_{\mathbf{a}}^n f) (\mathbf{J}_{\mathbf{a}}^{n-\alpha} g) + g(a)(f - f(a))D_{\mathbf{a}}^\alpha [1], \end{aligned}$$

where we have utilized the fact that for  $n \in \mathcal{N}$ ,  $D_{\mathbf{a}}^n = D^n = D_{\mathbf{a}}^k$ . □

## 1.4 Classical Fractional Derivatives

In one dimension, we present definitions and properties of fractional derivatives and integrals in this section. Interested readers are referred to the classical books (Kilbas et al. [52], Klimek [55], Podlubny [101], Samko et al. [110]) for details.

**Definition 1.4.1** (*Left and right Riemann–Liouville fractional integrals*) The left and right Riemann–Liouville fractional integrals  ${}_a\mathcal{I}_t^\alpha$  and  ${}_t\mathcal{I}_b^\alpha$  of order  $\alpha \in \mathbb{R}$ ,  $\alpha > 0$ , are defined, respectively, by

$${}_a\mathcal{I}_t^\alpha [f](t) = \frac{1}{\Gamma(\alpha)} \int_a^t \frac{f(\mu)d\mu}{(t-\mu)^{1-\alpha}}, \quad t \in (a, b],$$

and

$${}_t\mathcal{I}_b^\alpha [f](t) = \frac{1}{\Gamma(\alpha)} \int_t^b \frac{f(\mu)d\mu}{(t-\mu)^{1-\alpha}}, \quad t \in [a, b),$$

where  $\Gamma(\alpha)$  represents the Euler’s gamma function.

**Definition 1.4.2** (*Left and right Hadamard fractional integrals*) Assume  $0 \leq a < b, \infty$ . The left and right Hadamard fractional integrals of order  $\alpha \in \mathbb{R}$  for  $\alpha > 0$  are, respectively, given by

$${}_a\mathcal{I}_t^\alpha[f](t) = \frac{1}{\Gamma(\alpha)} \int_a^t \left(\log \frac{t}{\mu}\right)^{\alpha-1} \frac{f(\mu)d\mu}{\mu}, \quad t > a$$

and

$${}_t\mathcal{I}_b^\alpha[f](t) = \frac{1}{\Gamma(\alpha)} \int_t^b \left(\log \frac{t}{\mu}\right)^{\alpha-1} \frac{f(\mu)d\mu}{\mu}, \quad t < b.$$

In this section, we only define the Riemann–Liouville fractional derivatives of order  $\alpha$  in the interval  $0 < \alpha < 1$ . We refer our readers to Kilbas et al. [52] for a more general definition for any  $\alpha$  with  $Re(\alpha) > 0$ .

**Definition 1.4.3** (*Left and right Riemann–Liouville fractional derivatives*) The left and right Riemann–Liouville fractional derivative of order  $\alpha \in \mathbb{R}$  in the interval  $0 < \alpha < 1$  of a function  $f$ , denoted here by  ${}_a\mathcal{D}_t^\alpha[f]$ , is given by

$${}_a\mathcal{D}_t^\alpha[f](t) = \frac{d}{dt} {}_a\mathcal{I}_t^{1-\alpha}[f](t), \quad \text{for all } t \in (a, b).$$

In the same manner, the right Liouville fractional derivative of order  $\alpha \in \mathbb{R}$  in the interval  $0 < \alpha < 1$  of a function  $f$ , represented by  ${}_a\mathcal{D}_t^\alpha[f]$ , is defined by

$${}_t\mathcal{D}_b^\alpha[f](t) = -\frac{d}{dt} {}_t\mathcal{I}_b^{1-\alpha}[f](t), \quad \text{for all } t \in [a, b).$$

**Proposition 1.4.4** (Kilbas et al. [52], Malinowska et al. [80]) Assume  $\alpha > 0, \beta > 0$ . Then the following identities satisfies:

$$\begin{aligned} {}_a\mathcal{I}_t^\alpha [(\mu - a)^{\beta-1}] (t) &= \frac{\Gamma(\beta)}{\Gamma(\beta + \alpha)} (t - a)^{\beta+\alpha-1}, \\ {}_a\mathcal{D}_t^\alpha [(\mu - a)^{\beta-1}] (t) &= \frac{\Gamma(\beta)}{\Gamma(\beta - \alpha)} (t - a)^{\beta-\alpha-1}, \\ {}_a\mathcal{I}_b^\alpha [(b - \mu)^{\beta-1}] (t) &= \frac{\Gamma(\beta)}{\Gamma(\beta + \alpha)} (b - t)^{\beta+\alpha-1}, \quad \text{and} \\ {}_t\mathcal{D}_b^\alpha [(b - \mu)^{\beta-1}] (t) &= \frac{\Gamma(\beta)}{\Gamma(\beta - \alpha)} (b - t)^{\beta-\alpha-1} \end{aligned}$$

**Definition 1.4.5** (*The left and right Caputo fractional derivatives* [80]) The left and right Caputo fractional derivatives of order  $\alpha \in \mathbb{R}$  ( $0 < \alpha < 1$ ) are, respectively, defined by

$${}^c\mathcal{D}_t^\alpha[f](t) = {}_a\mathcal{I}_t^{1-\alpha} \left[ \frac{d}{dt} f \right] (t), \quad \text{for all } t \in (a, b)$$

and

$${}_t^C \mathcal{D}_b^\alpha [f](t) = {}_t \mathcal{I}_b^{1-\alpha} \left[ \frac{d}{dt} f \right] (t), \quad \text{for all } t \in [a, b).$$

In the spirits of [52, 80], we let  $\alpha \in (0, 1)$  and define function  $f \in \mathcal{C}([a, b]; \mathbb{R})$ , where  $\mathcal{C}$  stands for the class of absolutely continuous functions. Then the Caputo and Riemann–Liouville fractional derivatives hold for the relations

$${}_a^C \mathcal{D}_t^\alpha [f](t) = {}_a \mathcal{D}_t^\alpha [f](t) - \frac{f(a)}{(t-a)^\alpha \Gamma(1-\alpha)}, \quad (1.4.1)$$

$${}_t^C \mathcal{D}_b^\alpha [f](t) = {}_a \mathcal{D}_t^\alpha [f](t) + \frac{f(b)}{(b-t)^\alpha \Gamma(1-\alpha)}, \quad (1.4.2)$$

In addition for Riemann–Liouville fractional derivatives and integrals, the following rules are held

$$({}_a \mathcal{I}_t^\alpha \cdot {}_a \mathcal{D}_t^\alpha) [f](t) = f(t), \quad (1.4.3)$$

$$({}_t \mathcal{I}_b^\alpha \cdot {}_t \mathcal{D}_b^\alpha) [f](t) = f(t), \quad (1.4.4)$$

provided that  $f \in L^1(a, b; \mathbb{R})$ ,  ${}_a \mathcal{I}_t^\alpha [f]$ ,  ${}_t \mathcal{I}_b^\alpha [f] \in \mathcal{C}([-, \cdot]; \mathcal{R})$  and  ${}_a \mathcal{I}_t^\alpha f(a) = 0$ ,  ${}_t \mathcal{I}_b^\alpha f(b) = 0$ . It should be noted that if  $f(a) = 0$ , then from Eqs. (1.4.1) and (1.4.3) we have

$$({}_a \mathcal{I}_t^\alpha \cdot {}_a^C \mathcal{D}_t^\alpha) [f](t) = ({}_a \mathcal{I}_t^\alpha \cdot {}_a \mathcal{D}_t^\alpha) [f](t) = f(t),$$

similarly, with  $f(b) = 0$ , it implies from (1.4.2) and (1.4.4) that

$$({}_t \mathcal{I}_b^\alpha \cdot {}_t^C \mathcal{D}_b^\alpha) [f](t) = ({}_t \mathcal{I}_b^\alpha \cdot {}_t \mathcal{D}_b^\alpha) [f](t) = f(t).$$

To show that Riemann–Liouville fractional integrals hold for semi-group property, we make the following propositions.

**Proposition 1.4.6** (See Lemma 2.3, Kilbas et al. [52]) *Let  $\alpha, \beta > 0$  and  $f \in L^\gamma(a, b; \mathbb{R})$ , for  $1 \leq \gamma \leq \infty$ . Then equations*

$$({}_a \mathcal{I}_t^\alpha \cdot {}_a \mathcal{I}_t^\beta) [f](t) = {}_a \mathcal{I}_t^{\alpha+\beta} [f](t)$$

and

$$({}_t \mathcal{I}_b^\alpha \cdot {}_t \mathcal{I}_b^\beta) [f](t) = {}_t \mathcal{I}_b^{\alpha+\beta} [f](t)$$

are held in  $(a, b)$ .

In the following results, we show for some functions that the Caputo and Riemann–Liouville fractional derivatives are left inverse operators of Riemann–Liouville fractional integrals [52, 80].

**Proposition 1.4.7** *Let  $0 < \alpha < 1$  and  $f \in L^\gamma(a, b; \mathbb{R})$  for  $1 \leq \gamma \leq \infty$ , then the following*

$$\begin{aligned}({}_a \mathcal{D}_t^\alpha \cdot {}_a \mathcal{I}_t^\alpha)[f](t) &= f(t), \\({}_t \mathcal{D}_b^\alpha \cdot {}_t \mathcal{I}_b^\alpha)[f](t) &= f(t)\end{aligned}$$

*is satisfied in  $(a, b)$ .*

**Proposition 1.4.8** *Let  $0 < \alpha < 1$ . If  $f$  is continuous in  $[a, b]$ , then*

$$\begin{aligned}({}_a^C \mathcal{D}_t^\alpha \cdot {}_a \mathcal{I}_t^\alpha)[f](t) &= f(t), \\({}_t^C \mathcal{D}_b^\alpha \cdot {}_t \mathcal{I}_b^\alpha)[f](t) &= f(t).\end{aligned}$$

For  $\gamma$ -Lebesgue integrable functions (as given in Proposition 1.4.7), Riemann–Liouville derivatives and integral hold for the following properties.

**Proposition 1.4.9** (Kilbas et al. [52]) *Let  $0 < \beta < \alpha < 1$  and  $f \in L^\gamma(a, b; \mathbb{R})$  for  $1 \leq \gamma \leq \infty$ , then the following properties*

$$\begin{aligned}({}_a \mathcal{D}_t^\beta \cdot {}_a \mathcal{I}_t^{\alpha-\beta})[f](t) &= f(t), \\({}_t \mathcal{D}_b^\beta \cdot {}_t \mathcal{I}_b^{\alpha-\beta})[f](t) &= f(t)\end{aligned}$$

*are held in  $(a, b)$ .*

**Lemma 1.4.10** (Klimek [55]) *Let  $0 < \alpha < 1$  and functions  $f \in C([a, b]; \mathbb{R})$ ,  $g \in L^\gamma([a, b]; \mathbb{R})$  for  $1 \leq \gamma \leq \infty$ . Then, the integration by parts formula*

$$\int_a^b f(t) {}_a D_t^\alpha [g](t) dt = \int_a^b g(t) {}_a^C D_b^\alpha [f](t) dt + f(t) {}_a \mathcal{I}_t^{1-\alpha} [g](t) \Big|_{t=a}^{t=b}.$$

holds. Details proof is given in Lemma 2.19 of [55].

## 1.5 Partial Riemann–Liouville Fractional Derivative

Most studies on the anomalous diffusion are often carried out in one-dimensional space, see, for instance, [114, 126, 128] and references cited therein, where the involved Riemann–Liouville derivative is defined with order  $\alpha$  bounded in the open interval  $0 < \alpha < 1$  in one space dimension. The concern question will be: ‘if the anomalous diffusion phenomenon occurs in  $\mathbb{R}^2$  or in higher spatial dimensions, how do we go about its model’ or ‘how do one define the partial Riemann–Liouville derivative?’ We first introduce in this section, the partial Riemann–Liouville derivatives mentioned [66, 110], and then proceed to define the partial Caputo derivatives in a similar fashion.

Assume  $\alpha_i \in (0, 1)$ , for  $i = 1, 2$  and  $\alpha = \alpha_1 + \alpha_2$ . We define

$$\begin{aligned} {}_{RL}\partial_{x^{\alpha_1}y^{\alpha_2}}^{\alpha_1+\alpha_2}f(x, y) &= \frac{\partial^{\alpha_2}}{\partial y^{\alpha_2}} \left( \frac{\partial^{\alpha_1}}{\partial x^{\alpha_1}} f(x, y) \right) \\ &= \frac{\partial^{\alpha_2}}{\partial y^{\alpha_2}} \left( \frac{1}{\Gamma(1-\alpha_1)} \frac{\partial}{\partial x} \int_0^x (x-\tau)^{-\alpha_1} f(\tau, y) d\tau \right) \\ &= \frac{1}{\Gamma(1-\alpha_2)} \frac{\partial}{\partial y} \int_0^y \frac{(y-\xi)^{-\alpha_2}}{\Gamma(1-\alpha_1)} \frac{\partial}{\partial x} \int_0^x (x-\tau)^{-\alpha_1} f(\tau, \xi) d\tau d\xi, \end{aligned}$$

then

$${}_{RL}\partial_{x^{\alpha_1}y^{\alpha_2}}^{\alpha_1+\alpha_2}f(x, y) = \frac{1}{\Gamma(1-\alpha_1)\Gamma(1-\alpha_2)} \frac{\partial^2}{\partial x \partial y} \int_0^y \int_0^x (y-\xi)^{-\alpha_2} (x-\tau)^{-\alpha_1} f(\tau, \xi) d\tau d\xi.$$

Known from the classical calculus, if

$$\frac{\partial^2}{\partial x \partial y} \int_0^y \int_0^x (y-\xi)^{-\alpha_2} (x-\tau)^{-\alpha_1} f(\tau, \xi) d\tau d\xi$$

and

$$\frac{\partial^2}{\partial x \partial y} \int_0^y \int_0^x (y-\xi)^{-\alpha_2} (x-\tau)^{-\alpha_1} f(\tau, \xi) d\xi d\tau$$

exist and continuous in a neighbourhood of  $(x, y)$ , then

$${}_{RL}\partial_{x^{\alpha_1}y^{\alpha_2}}^{\alpha_1+\alpha_2}f(x, y) = {}_{RL}\partial_{y^{\alpha_2}x^{\alpha_1}}^{\alpha_1+\alpha_2}f(x, y).$$

*Remark 1.5.1* If  $\alpha = \alpha_1 + \alpha_2 \in (0, 1)$ , then the above partial Riemann–Liouville fractional derivative can be regarded as sub-diffusion type in  $\mathbb{R}^2$  [16, 96, 97].

The case which corresponds with  $\alpha_1 = 0$  or  $\alpha_2 = 0$  has been reported by Kilbas et al. [52],

$$\begin{aligned} {}_{RL}\partial_{y^{\alpha_2}}^{\alpha_2}f(x, y) &= \frac{\partial^{\alpha_2}}{\partial y^{\alpha_2}}f(x, y) = \frac{1}{\Gamma(1-\alpha_2)} \frac{\partial}{\partial y} \int_0^y (y-\xi)^{-\alpha_2} f(x, \xi) d\xi, \\ {}_{RL}\partial_{x^{\alpha_1}}^{\alpha_1}f(x, y) &= \frac{\partial^{\alpha_1}}{\partial x^{\alpha_1}}f(x, y) = \frac{1}{\Gamma(1-\alpha_1)} \frac{\partial}{\partial x} \int_0^x (x-\tau)^{-\alpha_1} f(x, \tau) d\tau. \end{aligned}$$

In what follows, we give the definition of the partial Riemann–Liouville fractional derivative.

**Definition 1.5.2** The partial Riemann–Liouville fractional derivative with order  $\alpha_1 + \alpha_2$ , where  $\alpha_1$  and  $\alpha_2$  are given in the directions  $x$  and  $y$ , respectively, are defined as follows:

$${}_{RL}\partial_{x^{\alpha_1} y^{\alpha_2}}^{\alpha_1+\alpha_2} f(x, y) = \frac{1}{\Gamma(p-\alpha_1)\Gamma(q-\alpha_2)} \frac{\partial^{p+q}}{\partial x^p \partial y^q} \times \int_0^y \int_0^x (y-\xi)^{q-\alpha_2-1} (x-\tau)^{p-\alpha_1-1} f(\tau, \xi) d\tau d\xi,$$

where  $\alpha_1 \in (p-1, p)$  and  $\alpha_2 \in (q-1, q)$ , for  $p, q \in \mathbb{Z}^+$ .

*Remark 1.5.3* If the derivative value of the integral in the right-hand side of the above equation has no relation to partial differential sequence, then the same is applicable to the left-hand side of the above equation.

In the following, we present the definition of a more higher spatial dimension.

**Definition 1.5.4** The partial Riemann–Liouville fractional derivative of order  $\sum_{i=1}^{\eta} \alpha_i$  in the direction  $x_i$ ,  $i = 1, 2, \dots, \eta$  is defined as

$${}_{RL}\partial_{x_1^{\alpha_1} \dots x_{\eta}^{\alpha_{\eta}}}^{\alpha_1+\dots+\alpha_{\eta}} f(x_1, x_2, \dots, x_{\eta}) = \frac{(\partial^{p_1} + \dots + \partial^{p_{\eta}})/(\partial x_1^{p_1} \dots \partial x_{\eta}^{p_{\eta}})}{\prod_{i=1}^{\eta} \Gamma(p_i - \alpha_i)} \times \int_0^{x_{\eta}} \dots \int_0^{x_1} (x_{\eta} - \tau_{\eta})^{p_{\eta}-\alpha_{\eta}-1} \dots (x_1 - \tau_1)^{p_1-\alpha_1-1} f d\tau_1 \dots d\tau_{\eta},$$

where  $\alpha_i \in (p_i - 1, p_i)$ ,  $p_i \in \mathbb{Z}^+$ ,  $i = 1, 2, \dots, \eta$ .

With reference to the work by Li and Deng [68], it is not difficult to show that

$$\lim_{\alpha_i \rightarrow p_i^-} \partial_{x_1^{\alpha_1} \dots x_{\eta}^{\alpha_{\eta}}}^{\alpha_1+\dots+\alpha_{\eta}} f(x_1, x_2, \dots, x_{\eta}) = {}_{RL}\partial_{x_1^{\alpha_1} \dots x_{i-1}^{\alpha_{i-1}} x_{i+1}^{\alpha_{i+1}} \dots x_{\eta}^{\alpha_{\eta}}}^{\alpha_1+\dots+\alpha_{i-1}+\alpha_{i+1}+\dots+\alpha_{\eta}} \frac{\partial^{p_i}}{\partial x_i^{p_i}} f(x_1, x_2, \dots, x_{\eta}),$$

and

$$\lim_{\alpha_i \rightarrow (p_i-1)^+} \partial_{x_1^{\alpha_1} \dots x_{\eta}^{\alpha_{\eta}}}^{\alpha_1+\dots+\alpha_{\eta}} f(x_1, x_2, \dots, x_{\eta}) = {}_{RL}\partial_{x_1^{\alpha_1} \dots x_{i-1}^{\alpha_{i-1}} x_{i+1}^{\alpha_{i+1}} \dots x_{\eta}^{\alpha_{\eta}}}^{\alpha_1+\dots+\alpha_{i-1}+\alpha_{i+1}+\dots+\alpha_{\eta}} \frac{\partial^{p_i-1}}{\partial x_i^{p_i-1}} f(x_1, x_2, \dots, x_{\eta}).$$

Next, we can now define the Caputo partial fractional derivative by following a similar process.

**Definition 1.5.5** Two-dimensional type: the Caputo partial fractional derivative of order  $\alpha_1 + \alpha_2$  in the directions  $(x, y)$  which correspond to order  $(\alpha_1, \alpha_2)$ , respectively, is defined by

$${}_{C}\partial_{x^{\alpha_1} y^{\alpha_2}}^{\alpha_1+\alpha_2} f(x, y) = \frac{1}{\Gamma(p-\alpha_1)\Gamma(q-\alpha_2)} \int_0^y \int_0^x (y-\xi)^{q-\alpha_2-1} (x-\tau)^{p-\alpha_1-1} \times \frac{\partial^{p+q}}{\partial \tau^p \partial \xi^q} f(\tau, \xi) d\tau d\xi,$$

where  $\alpha_1 \in (p-1, p)$ ,  $\alpha_2 \in (q-1, q)$ ,  $p, q \in \mathbb{Z}^+$ .

**Definition 1.5.6** Higher dimensional type: the Caputo partial fractional derivative with order  $\sum_{i=1}^{\tau} \alpha_i$ , for  $\alpha_i$ th order in  $x_i$ -direction,  $i = 1, 2, \dots, \tau$  is defined by

$${}_C \partial_{x_1^{\alpha_1}, \dots, x_{\eta}^{\alpha_{\eta}}}^{\alpha_1 + \dots + \alpha_{\eta}} f(x_1, \dots, x_{\eta}) = \frac{1}{\prod_{i=1}^{\eta} \Gamma(p_i - \alpha_i)} \times \int_0^{x_{\eta}} \dots \int_0^{x_1} (x_{\eta} - \tau_{\eta})^{p_{\eta} - \alpha_{\eta} - 1} \dots (x_1 - \tau_1)^{p_1 - \alpha_1 - 1} \frac{\partial^{p_1} + \dots + p_{\eta}}{\partial \tau_1^{p_1} \dots \partial \tau_{\eta}^{p_{\eta}}} f(\tau_1, \dots, \tau_{\eta}) d\tau_1 \dots d\tau_{\eta},$$

where  $\alpha_i \in (p_i - 1, p_i)$ ,  $p_i \in \mathbb{Z}^+$ ,  $i = 1, 2, \dots, \tau$ .

*Remark 1.5.7* If the derivative values of the integrals in the right-hand sides of the equalities in above definitions do not relate to partial differential sequence, so also the values of the left-hand sides do not either.

One can also obtain

$$\lim_{\alpha_i \rightarrow p_i^-} {}_C \partial_{x_1^{\alpha_1}, \dots, x_{\eta}^{\alpha_{\eta}}}^{\alpha_1 + \dots + \alpha_{\eta}} f(x_1, \dots, x_{\eta}) = {}_C \partial_{x_1^{\alpha_1}, \dots, x_{i-1}^{\alpha_{i-1}}, x_{i+1}^{\alpha_{i+1}}, \dots, x_{\eta}^{\alpha_{\eta}}}^{\alpha_1 + \dots + \alpha_{i-1} + \alpha_{i+1} + \dots + \alpha_{\eta}} \frac{\partial^{p_i}}{\partial x_i^{p_i}} f(x_1, x_2, \dots, x_{\eta}),$$

and

$$\begin{aligned} \lim_{\alpha_i \rightarrow (p_i - 1)^+} {}_C \partial_{x_1^{\alpha_1}, \dots, x_{\eta}^{\alpha_{\eta}}}^{\alpha_1 + \dots + \alpha_{\eta}} f(x_1, \dots, x_{\eta}) &= {}_C \partial_{x_1^{\alpha_1}, \dots, x_{i-1}^{\alpha_{i-1}}, x_{i+1}^{\alpha_{i+1}}, \dots, x_{\eta}^{\alpha_{\eta}}}^{\alpha_1 + \dots + \alpha_{i-1} + \alpha_{i+1} + \dots + \alpha_{\eta}} \frac{\partial^{p_i - 1}}{\partial x_i^{p_i - 1}} f(x_1, x_2, \dots, x_{\eta}) \\ &\quad - {}_C \partial_{x_1^{\alpha_1}, \dots, x_{i-1}^{\alpha_{i-1}}, x_{i+1}^{\alpha_{i+1}}, \dots, x_{\eta}^{\alpha_{\eta}}}^{\alpha_1 + \dots + \alpha_{i-1} + \alpha_{i+1} + \dots + \alpha_{\eta}} \frac{\partial^{p_i - 1}}{\partial x_i^{p_i - 1}} f(x_1, \dots, x_{i-1}, 0, x_{i+1}, \dots, x_{\eta}). \end{aligned}$$

**Definition 1.5.8** The Riemann–Liouville partial integral with fractional-order  $\sum_{i=1}^{\eta} \alpha_i$  (for order  $\alpha_i$ th in the direction  $x_i$ ,  $i = 1, 2, \dots, \tau$ ) is defined as

$${}_{RL} \partial_{x_1^{\alpha_1}, \dots, x_{\eta}^{\alpha_{\eta}}}^{\alpha_1 + \dots + \alpha_{\eta}} f(x_1, \dots, x_{\tau}) = \frac{1}{\prod_{i=1}^{\eta} \Gamma(\alpha_i)} \int_0^{x_{\eta}} \dots \int_0^{x_1} (x_{\eta} - \tau_{\eta})^{\alpha_{\eta} - 1} \dots (x_1 - \tau_1)^{\alpha_1 - 1} f d\tau_1 \dots d\tau_{\eta},$$

where  $\alpha_i \in \mathbb{R}^+$ ,  $i = 1, \dots, \tau$ .

## 1.6 Fractional Operators with Variable Order

The study of fractional differentiation and integration for a non constant order was proposed in 1993 in a pioneering paper written by Samko and Ross [109]. The study which had since generated a lot of research attention based on reports dedicated to fractional operators with variable orders as well as their applications, (see,

for instance, Almeida and Samko [5], Coimbra [24], Lorenzo and Hartley [74], Ma et al. [76], Malinowska et al. [80], Odziejewicz et al. [90, 91] and Tavares et al. [116] ). In 2009, Diaz and Coimbra [29] proposed two controllers for the variable order differential equations that can handle an arbitrary reference function. A variable order differential equation for a particle in a quiescent viscous medium was developed by Ramirez and Coimbra [104]. For details on the application of fractional operators with variable order to the modelling of dynamic systems, readers are referred to the books and articles [80, 103, 110, 116].

Our interest here is to first consider a situation where the fractional derivative of variable order  $\alpha$  is treated as a function of time, that is,  $\alpha(t)$  on the open interval  $0 < \alpha(t) < 1$ . To begin, we present different types of Riemann–Liouville fractional derivatives of variable order  $\alpha(t) \in (0, 1)$ .

**Definition 1.6.1** (In Riemann–Liouville sense, the left and right fractional derivatives of variable order  $\alpha(t)$  for types I and II). Given a function  $f : [a, b] \rightarrow \mathbb{R}$ ,

(i) the left Riemann–Liouville type-I fractional derivative of order  $\alpha(t)$  is given by

$${}_a\mathcal{D}_t^{\alpha(t)} f(t) = \frac{1}{\Gamma(1 - \alpha(t))} \frac{d}{dt} \int_a^t (t - \tau)^{-\alpha(t)} f(\tau) d\tau,$$

(ii) the right Riemann–Liouville type-I fractional derivative of order  $\alpha(t)$  is defined by

$${}_t\mathcal{D}_b^{\alpha(t)} f(t) = \frac{-1}{\Gamma(1 - \alpha(t))} \frac{d}{dt} \int_t^b (t - \tau)^{-\alpha(t)} f(\tau) d\tau,$$

(iii) the left Riemann–Liouville type-II fractional derivative of order  $\alpha(t)$  is defined by

$${}_a\mathbb{D}_t^{\alpha(t)} f(t) = \frac{d}{dt} \left( \frac{1}{\Gamma(1 - \alpha(t))} \int_a^t (t - \tau)^{-\alpha(t)} f(\tau) d\tau \right),$$

(iv) the right Riemann–Liouville type-II fractional derivative of order  $\alpha(t)$  is defined by

$${}_t\mathbb{D}_b^{\alpha(t)} f(t) = \frac{d}{dt} \left( \frac{-1}{\Gamma(1 - \alpha(t))} \int_t^b (\tau - t)^{-\alpha(t)} f(\tau) d\tau \right).$$

**Definition 1.6.2** (In Caputo sense, the left and right fractional derivatives of variable order  $\alpha(t)$  for types I, II and III). Given a function  $f : [a, b] \rightarrow \mathbb{R}$ ,

(i) the left Caputo type-I fractional derivative of order  $\alpha(t)$  is given by

$${}_a^C\mathcal{D}_t^{\alpha(t)} f(t) = {}_a^C\mathcal{D}_t^{\alpha(t)} [f(t) - f(a)] = \frac{1}{\Gamma(1 - \alpha(t))} \frac{d}{dt} \int_a^t (t - \tau)^{-\alpha(t)} [f(\tau) - f(a)] d\tau,$$

(ii) the right Caputo type-I fractional derivative of order  $\alpha(t)$  is given by

$${}_t^C\mathcal{D}_b^{\alpha(t)} f(t) = {}_t^C\mathcal{D}_b^{\alpha(t)} [f(t) - f(b)] = \frac{-1}{\Gamma(1 - \alpha(t))} \frac{d}{dt} \int_t^b (\tau - t)^{-\alpha(t)} [f(\tau) - f(b)] d\tau,$$

(iii) the left Caputo type-II fractional derivative of order  $\alpha(t)$  is defined by

$${}_a^C \mathbb{D}_t^{\alpha(t)} f(t) = {}_a^C \mathbb{D}_t^{\alpha(t)} [f(t) - f(a)] = \frac{d}{dt} \left( \frac{1}{\Gamma(1 - \alpha(t))} \int_a^t (t - \tau)^{-\alpha(t)} [f(\tau) - f(a)] d\tau \right),$$

(iv) the right Caputo type-II fractional derivative of order  $\alpha(t)$  is defined by

$${}_t^C \mathbb{D}_b^{\alpha(t)} f(t) = {}_t^C \mathbb{D}_b^{\alpha(t)} [f(t) - f(b)] = \frac{d}{dt} \left( \frac{-1}{\Gamma(1 - \alpha(t))} \int_t^b (\tau - t)^{-\alpha(t)} [f(\tau) - f(b)] d\tau \right),$$

(v) the left Caputo type-III fractional derivative of order  $\alpha(t)$  is defined by

$${}_a^C \mathcal{D}_t^{\alpha(t)} f(t) = \frac{1}{\Gamma(1 - \alpha(t))} \int_a^t (t - \tau)^{-\alpha(t)} f'(\tau) d\tau,$$

(vi) the right Caputo type-III fractional derivative of order  $\alpha(t)$  is defined by

$${}_t^C \mathcal{D}_b^{\alpha(t)} f(t) = \frac{1}{\Gamma(1 - \alpha(t))} \int_t^b (\tau - t)^{-\alpha(t)} f'(\tau) d\tau.$$

**Theorem 1.6.3** *The following relations are satisfied between the left fractional operators:*

$${}_a^C \mathcal{D}_t^{\alpha(t)} f(t) = {}_a^C \mathbb{D}_t^{\alpha(t)} f(t) + \frac{\alpha'(t)}{\Gamma(2 - \alpha(t))} \int_a^t (t - \tau)^{1 - \alpha(t)} f'(\tau) \left( \frac{1}{1 - \alpha(t)} - \ln(t - \tau) \right) d\tau \quad (1.6.1)$$

and

$${}_a^C \mathcal{D}_t^{\alpha(t)} f(t) = {}_a^C \mathcal{D}_t^{\alpha(t)} f(t) - \frac{\alpha'(t) \Phi(1 - \alpha(t))}{\Gamma(1 - \alpha(t))} \int_a^t (t - \tau)^{-\alpha(t)} [f(\tau) - f(a)] d\tau. \quad (1.6.2)$$

*Proof* On integrating by parts, one obtains

$$\begin{aligned} {}_a^C \mathcal{D}_t^{\alpha(t)} f(t) &= \frac{1}{\Gamma(1 - \alpha(t))} \frac{d}{dt} \int_a^t (t - \tau)^{-\alpha(t)} [f(\tau) - f(a)] d\tau \\ &= \frac{1}{\Gamma(1 - \alpha(t))} \frac{d}{dt} \left[ \frac{1}{1 - \alpha(t)} \int_a^t (t - \tau)^{1 - \alpha(t)} f'(\tau) d\tau \right]. \end{aligned}$$

It follows from differentiating the integral that

$$\begin{aligned} {}_a^C \mathcal{D}_t^{\alpha(t)} f(t) &= \frac{1}{\Gamma(1 - \alpha(t))} \left[ \frac{\alpha'(t)}{(1 - \alpha(t))^2} \int_a^t (t - \tau)^{1 - \alpha(t)} f'(\tau) d\tau \right. \\ &\quad \left. + \frac{1}{1 - \alpha(t)} \int_a^t (t - \tau)^{1 - \alpha(t)} f'(\tau) \left( -\alpha'(t) \ln(t - \tau) + \frac{1 - \alpha(t)}{t - \tau} \right) d\tau \right] \\ &= {}_a^C \mathcal{D}_t^{\alpha(t)} f(t) + \frac{\alpha'(t)}{\Gamma(2 - \alpha(t))} \int_a^t (t - \tau)^{1 - \alpha(t)} f'(\tau) \left[ \frac{1}{1 - \alpha(t)} - \ln(t - \tau) \right] d\tau. \end{aligned}$$

For the second formula, it also follows from direct calculations. Hence, we can deduce that when the order  $\alpha(t)$  is equal to a constant, say  $c$ , we have  ${}^C_a\mathcal{D}_t^{\alpha(t)} f(t) = {}^C_a\mathbb{D}_t^{\alpha(t)} f(t) = {}^C_a D_t^{\alpha(t)} f(t)$ .  $\square$

In a similar manner, we obtain the following result.

**Theorem 1.6.4** *The following relations are satisfied between the right fractional operators:*

$${}^C_a\mathcal{D}_b^{\alpha(t)} f(t) = {}^C_a D_b^{\alpha(t)} f(t) + \frac{\alpha'(t)}{\Gamma(2-\alpha(t))} \int_t^b (\tau-t)^{1-\alpha(t)} f'(\tau) \left( \frac{1}{1-\alpha(t)-\ln(\tau-t)} \right) d\tau$$

and

$${}^C_b\mathcal{D}_b^{\alpha(t)} f(t) = {}^C_b\mathbb{D}_b^{\alpha(t)} f(t) + \frac{\alpha'(t)\Phi(1-\alpha(t))}{\Gamma(1-\alpha(t))} \int_t^b (\tau-t)^{-\alpha(t)} [f(\tau) - f(b)] d\tau.$$

**Theorem 1.6.5** *Let  $f \in C^1([a, b], \mathbb{R})$ . At  $t = a$*

$${}^C_a\mathcal{D}_t^{\alpha(t)} f(t) = {}^C_a\mathbb{D}_t^{\alpha(t)} f(t) = {}^C_a D_t^{\alpha(t)} f(t) = 0,$$

while at  $t = b$

$${}^C_b\mathcal{D}_b^{\alpha(t)} f(t) = {}^C_b\mathbb{D}_b^{\alpha(t)} f(t) = {}^C_b D_b^{\alpha(t)} f(t) = 0.$$

*Proof* At initial time  $t = a$  for the third equality, we note that

$$\left| {}^C_a\mathcal{D}_t^{\alpha(t)} f(t) \right| \leq \frac{\|f'\|}{\Gamma(1-\alpha(t))} \int_a^t (t-\tau)^{-\alpha(t)} d\tau = \frac{\|f'\|}{\Gamma(2-\alpha(t))} (t-a)^{1-\alpha(t)}$$

which at  $t = a$  is zero. By considering the first equality using Eq. (1.6.1) at  $t = a$ , and the next two relations

$$\left| \int_a^t (t-\tau)^{1-\alpha(t)} \frac{f'(\tau)}{1-\alpha(t)} d\tau \right| \leq \frac{\|f'\|}{(1-\alpha(t))(2-\alpha(t))} (t-a)^{2-\alpha(t)}$$

and

$$\left| \int_a^t (t-\tau)^{-\alpha(t)} f'(\tau) \ln(t-\tau) d\tau \right| \leq \frac{\|f'\|}{2-\alpha(t)} (t-a)^{2-\alpha(t)} \left| \ln(t-a) - \frac{1}{2-\alpha(t)} \right|,$$

integration by parts is used to get the latter equality, we prove that  ${}^C_a\mathcal{D}_t^{\alpha(t)} f(t) = 0$  at initial time  $t = a$ . The above process is repeated for Eq. (1.6.2) at initial time  $t = a$ : which by adopting an integration by parts techniques, we obtain

$$\left| \int_a^t (t-\tau)^{-\alpha(t)} [f(\tau) - f(a)] d\tau \right| \leq \frac{\|f'\|}{(1-\alpha(t))(2-\alpha(t))} (t-a)^{2-\alpha(t)},$$

so  ${}^C_a\mathbb{D}_t^{\alpha(t)} f(t) = 0$  at time  $t = a$ . For the right fractional operators, the proof follows same arguments at time  $t = b$ .  $\square$

Relationship between the Riemann–Liouville and Caputo derivatives have been deduced with some computations, see [116]. For the left fractional operator, we have

$$\begin{aligned} {}_a\mathcal{D}_t^{\alpha(t)} f(t) &= {}^C_a\mathcal{D}_t^{\alpha(t)} f(t) + \frac{f(a)}{\Gamma(1 - \alpha(t))} \frac{d}{dt} \int at(t - \tau)^{-\alpha(t)} d\tau \\ &= {}^C_a\mathcal{D}_t^{\alpha(t)} f(t) + \frac{f(a)}{\Gamma(1 - \alpha(t))} (t - a)^{-\alpha(t)} + \frac{f(a)\alpha'(t)}{\Gamma(2 - \alpha(t))} (t - a)^{1-\alpha(t)} \\ &\quad \times \left[ \frac{1}{1 - \alpha(t)} - \ln(t - a) \right] \end{aligned}$$

and

$$\begin{aligned} {}_a\mathbb{D}_t^{\alpha(t)} f(t) &= {}^C_a\mathbb{D}_t^{\alpha(t)} f(t) + f(a) \frac{d}{dt} \left( \frac{1}{\Gamma(1 - \alpha(t))} \int_a^t (t - \tau)^{-\alpha(t)} d\tau \right) \\ &= {}^C_a\mathbb{D}_t^{\alpha(t)} f(t) + \frac{f(a)}{\Gamma(1 - \alpha(t))} (t - a)^{-\alpha(t)} + \frac{f(a)\alpha'(t)}{\Gamma(2 - \alpha(t))} (t - a)^{1-\alpha(t)} \\ &\quad \times [\Phi(2 - \alpha(t)) - \ln(t - a)]. \end{aligned}$$

Also, for the right fractional operators, we obtain

$$\begin{aligned} {}_t\mathcal{D}_b^{\alpha(t)} f(t) &= {}^C_t\mathcal{D}_b^{\alpha(t)} f(t) + \frac{f(b)}{\Gamma(1 - \alpha(t))} (b - t)^{-\alpha(t)} \\ &\quad - \frac{f(b)\alpha'(t)}{\Gamma(2 - \alpha(t))} (b - t)^{1-\alpha(t)} \left[ \frac{1}{1 - \alpha(t)} - \ln(b - t) \right] \end{aligned}$$

and

$$\begin{aligned} {}_t\mathbb{D}_b^{\alpha(t)} f(t) &= {}^C_t\mathbb{D}_b^{\alpha(t)} f(t) + \frac{f(b)}{\Gamma(1 - \alpha(t))} (b - t)^{-\alpha(t)} \\ &\quad - \frac{f(b)\alpha'(t)}{\Gamma(2 - \alpha(t))} (b - t)^{1-\alpha(t)} [\Phi(2 - \alpha(t)) - \ln(b - t)]. \end{aligned}$$

Therefore, one can conclude that if  $f(a) = 0$ , then

$${}_a\mathcal{D}_t^{\alpha(t)} f(t) = {}^C_a\mathcal{D}_t^{\alpha(t)} f(t) \quad \text{and} \quad {}_a\mathbb{D}_t^{\alpha(t)} f(t) = {}^C_a\mathbb{D}_t^{\alpha(t)} f(t)$$

and likewise, if  $f(b) = 0$ , then

$${}_t\mathcal{D}_b^{\alpha(t)} f(t) = {}^C_t\mathcal{D}_b^{\alpha(t)} f(t) \quad \text{and} \quad {}_t\mathbb{D}_b^{\alpha(t)} f(t) = {}^C_t\mathbb{D}_b^{\alpha(t)} f(t).$$

In the next result, we formulate the Caputo fractional derivative of a power function.

**Corollary 1.6.6** *Let  $f(t) = (t - a)^\beta$  with  $\beta > 0$ . Then*

$$\begin{aligned} {}^C D_t^{\alpha(t)} f(t) &= \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha(t) + 1)} (t - a)^{\beta - \alpha(t)} - \alpha'(t) \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha(t) + 2)} (t - a)^{\beta - \alpha(t) + 1} \\ &\quad \times [\ln(t - a) - \Phi(\beta - \alpha(t) + 2) + \Phi(1 - \alpha(t))], \\ {}^C \mathbb{D}_t^{\alpha(t)} f(t) &= \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha(t) + 1)} (t - a)^{\beta - \alpha(t)} - \alpha'(t) \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha(t) + 2)} (t - a)^{\beta - \alpha(t) + 1} \\ &\quad \times [\ln(t - a) - \Phi(\beta - \alpha(t) + 2)], \\ {}^C D_t^{\alpha(t)} f(t) &= \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha(t) + 1)} (t - a)^{\beta - \alpha(t)}. \end{aligned}$$

*Proof* The expression for  ${}^C D_t^{\alpha(t)} f(t)$  if directly follows from [109, 116]. for the second equality, we have

$$\begin{aligned} {}^C \mathbb{D}_t^{\alpha(t)} f(t) &= \frac{d}{dt} \left( \frac{1}{\Gamma(1 - \alpha(t))} \int_a^t (t - \tau)^{-\alpha(t)} (\tau - a)^\beta d\tau \right) \\ &= \frac{d}{dt} \left( \frac{1}{\Gamma(1 - \alpha(t))} \int_a^t (t - a)^{-\alpha(t)} \left( 1 - \frac{\tau - a}{t - a} \right)^{-\alpha(t)} (\tau - a)^\beta d\tau \right). \end{aligned}$$

By introducing a change of variables  $\tau - a = x(t - a)$ , and with the assistance of the beta function  $\mathcal{B}(\cdot, \cdot)$ , we show that

$$\begin{aligned} {}^C \mathbb{D}_t^{\alpha(t)} f(t) &= \frac{d}{dt} \left( \frac{(t - a)^{-\alpha(t)}}{\Gamma(1 - \alpha(t))} \int_0^1 (1 - x)^{-\alpha(t)} x^\beta (t - a)^{\beta + 1} dx \right) \\ &= \frac{d}{dt} \left( \frac{(t - a)^{\beta - \alpha(t) + 1}}{\Gamma(1 - \alpha(t))} \mathcal{B}(\beta + 1, 1 - \alpha(t)) \right) \\ &= \frac{d}{dt} \left( \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha(t) + 2)} (t - a)^{\beta - \alpha(t) + 1} \right). \end{aligned}$$

By differentiating the latter expression, we obtain the desired formula. The same process hold for the last equality.  $\square$

The right Caputo fractional derivatives of variable order are simply obtained with analogous relations to those of Corollary 1.6.6.

**Corollary 1.6.7** *Let  $f(t) = (b - t)^\beta$  with  $\beta > 0$ . Then*

$$\begin{aligned} {}^C D_b^{\alpha(t)} f(t) &= \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha(t) + 1)} (b - t)^{\beta - \alpha(t)} + \alpha'(t) \frac{\Gamma(\beta + 1)}{\Gamma(\beta - \alpha(t) + 2)} (b - t)^{\beta - \alpha(t) + 1} \\ &\quad \times [\ln(b - t) - \Phi(\beta - \alpha(t) + 2) + \Phi(1 - \alpha(t))], \end{aligned}$$

$$\begin{aligned} {}_t^C \mathbb{D}_b^{\alpha(t)} f(t) &= \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha(t)+1)} (b-t)^{\beta-\alpha(t)} + \alpha'(t) \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha(t)+2)} (b-t)^{\beta-\alpha(t)+1} \\ &\quad \times [\ln(b-t) - \Phi(\beta-\alpha(t)+2)], \\ {}_t^C D_b^{\alpha(t)} f(t) &= \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha(t)+1)} (b-t)^{\beta-\alpha(t)}. \end{aligned}$$

The prove of the above Corollary follows a similar fashion with that of Corollary 1.6.6. With Corollary 1.6.6 in mind, it is not difficult to see that  ${}_a^C \mathcal{D}_t^{\alpha(t)} f(t) \neq {}_a^C \mathbb{D}_t^{\alpha(t)} f(t) \neq {}_a^C D_t^{\alpha(t)} f(t)$ . Also for the power function, it is clear that  ${}_a^C \mathcal{D}_t^{\alpha(t)}$  can be regarded as the best inverse operation for the fractional integral of variable order.

**Definition 1.6.8** (*Caputo partial fractional derivatives with variable order types I, II and III*) Partial fractional derivative are seen as a natural extension and are defined in a similar fashion. Given a function  $f : \prod_{i=1}^m [a_i, b_i] \rightarrow \mathbb{R}$  with  $m$  variables. For simplicity, we define the vectors  $|\tau|_s = (t_1, t_2, \dots, t_{s-1}, \tau, t_{s+1}, \dots, t_m) \in \mathbb{R}^m$  and denote  $(t^*) = (t_1, t_2, \dots, t_m) \in \mathbb{R}^m$ , fractional orders  $\alpha_s : [a_s, b_s] \rightarrow (0, 1)$ ,  $s \in \{1, 2, \dots, m\}$ ,

- (i) the type-I left Caputo partial fractional derivative of order  $\alpha_s(t_s)$  is defined by

$${}_{a_s}^C \mathcal{D}_{t_s}^{\alpha_s(t_s)} f(t^*) = \frac{1}{\Gamma(1-\alpha_s(t_s))} \frac{\partial}{\partial t_s} \int_{a_s}^{t_s} (t_s - \tau)^{-\alpha_s(t_s)} (f|_{\tau|_s} - f|_{a_s|_s}) d\tau,$$

- (ii) the type-I right Caputo partial fractional derivative of order  $\alpha_s(t_s)$  is defined by

$${}_{t_s}^C \mathcal{D}_{b_s}^{\alpha_s(t_s)} f(t^*) = \frac{-1}{\Gamma(1-\alpha_s(t_s))} \frac{\partial}{\partial t_s} \int_{t_s}^{b_s} (\tau - t_s)^{-\alpha_s(t_s)} (f|_{\tau|_s} - f|_{b_s|_s}) d\tau,$$

- (iii) the type-II left Caputo partial fractional derivative of order  $\alpha_s(t_s)$  is defined by

$${}_{a_s}^C \mathbb{D}_{t_s}^{\alpha_s(t_s)} f(t^*) = \frac{\partial}{\partial t_s} \left[ \frac{1}{\Gamma(1-\alpha_s(t_s))} \int_{a_s}^{t_s} (t_s - \tau)^{-\alpha_s(t_s)} (f|_{\tau|_s} - f|_{a_s|_s}) d\tau \right],$$

- (iv) the type-II right Caputo partial fractional derivative of order  $\alpha_s(t_s)$  is defined by

$${}_{t_s}^C \mathbb{D}_{b_s}^{\alpha_s(t_s)} f(t^*) = \frac{\partial}{\partial t_s} \left[ \frac{-1}{\Gamma(1-\alpha_s(t_s))} \int_{t_s}^{b_s} (\tau - t_s)^{-\alpha_s(t_s)} (f|_{\tau|_s} - f|_{b_s|_s}) d\tau \right],$$

- (v) the type-III left Caputo partial fractional derivative of order  $\alpha_s(t_s)$  is defined by

$${}_{a_s}^C D_{t_s}^{\alpha_s(t_s)} f(t^*) = \frac{1}{\Gamma(1-\alpha_s(t_s))} \int_{a_s}^{t_s} (t_s - \tau)^{-\alpha_s(t_s)} \frac{\partial f}{\partial t_s} [\tau]_s d\tau,$$

(vi) the type-III right Caputo partial fractional derivative of order  $\alpha_s(t_s)$  is defined by

$${}^C D_{t_s}^{\alpha_s(t_s)} f(t^*) = \frac{-1}{\Gamma(1 - \alpha_s(t_s))} \int_{a_s}^{t_s} (\tau - t_s)^{-\alpha_s(t_s)} \frac{\partial f}{\partial t_s} [\tau]_s d\tau.$$

As done before, we can prove the relations between these definitions in the same manner.

**Theorem 1.6.9** *The following formulas hold:*

$$\begin{aligned} {}^C \mathcal{D}_{t_s}^{\alpha_s(t_s)} f(t^*) &= {}^C D_{t_s}^{\alpha_s(t_s)} f(t^*) + \frac{\alpha'_s(t_s)}{\Gamma(2 - \alpha_s(t_s))} \int_{a_s}^{t_s} (t_s - \tau)^{1 - \alpha_s(t_s)} \frac{\partial f}{\partial t_s} [\tau]_s \\ &\quad \times \left[ \frac{1}{1 - \alpha_s(t_s)} - \ln(t_s - \tau) \right] d\tau, \end{aligned}$$

$${}^C \mathcal{D}_{a_s}^{\alpha_s(t_s)} f(t^*) = {}^C \mathbb{D}_{a_s}^{\alpha_s(t_s)} f(t^*) - \frac{\alpha'_s(t_s) \Phi(1 - \alpha_s(t_s))}{\Gamma(1 - \alpha_s(t_s))} \int_{a_s}^{t_s} (t_s - \tau)^{-\alpha_s(t_s)} [f[\tau]_s - f[a_s]_s] d\tau,$$

$$\begin{aligned} {}^C \mathcal{D}_{b_s}^{\alpha_s(t_s)} f(t^*) &= {}^C D_{b_s}^{\alpha_s(t_s)} f(t^*) + \frac{\alpha'_s(t_s)}{\Gamma(2 - \alpha_s(t_s))} \int_{t_s}^{b_s} (\tau - t_s)^{1 - \alpha_s(t_s)} \frac{\partial f}{\partial t_s} [\tau]_s \\ &\quad \times \left[ \frac{1}{1 - \alpha_s(t_s)} - \ln(\tau - t_s) \right] d\tau, \end{aligned}$$

and

$${}^C \mathcal{D}_{b_s}^{\alpha_s(t_s)} f(t^*) = {}^C \mathbb{D}_{b_s}^{\alpha_s(t_s)} f(t^*) - \frac{\alpha'_s(t_s) \Phi(1 - \alpha_s(t_s))}{\Gamma(1 - \alpha_s(t_s))} \int_{t_s}^{b_s} (\tau - t_s)^{-\alpha_s(t_s)} [f[\tau]_s - f[b_s]_s] d\tau.$$

In what follows, we briefly present the approximation of variable order derivatives in Caputo sense. Let  $q \in \mathbb{N}$ , we define

$$\begin{aligned} X_q &= \frac{1}{\Gamma(q + 1 - \alpha_s(t_s))} \left[ 1 + \sum_{k=n-q+1}^N \frac{\Gamma(\alpha_s(t_s) - n + k)}{\Gamma(\alpha_s(t_s) - q)(k - n + q)!} \right], \\ M_q(t^*) &= \max_{\tau \in [a_s, t_s]} \left| \frac{\partial^q f}{\partial t_s^q} [\tau]_s \right|, \\ Y_q &= \frac{\Gamma(\alpha_s(t_s) - n + q)}{\Gamma(1 - \alpha_s(t_s)) \Gamma(\alpha_k(t_k))(q - n)!}, \\ Z_q(t^*) &= \int_{a_s}^{t_s} (\tau - a_s)^{q-n} \frac{\partial f}{\partial t_s} [\tau]_s d\tau. \end{aligned}$$

**Theorem 1.6.10** *Let  $f \in C^{n+1}(\prod_{i=1}^m [a_i, b_i], \mathbb{R})$  with  $n \in \mathbb{N}$ . Then, for all  $s \in \{1, 2, \dots, m\}$  and for all  $N \in \mathbb{N}$  such that  $N \geq n$ , we have*

$${}^C_{a_s} D_{t_s}^{\alpha_s(t_s)} f(t^*) = \sum_{q=1}^n X_q (t_s - a_s)^{q-\alpha_s(t_s)} \frac{\partial^q f}{\partial t_s^q} [t_s]_s + \sum_{q=n}^N Y_q (t_s - a_s)^{n-q-\alpha_s(t_s)} Z_q(t^*) + \mathcal{E}(t^*),$$

with approximation error  $\mathcal{E}(t^*)$  bounded by

$$\mathcal{E}(t^*) \leq M_{n+1}(t^*) \frac{\exp[(n - \alpha_s(t_s))^2 + n - \alpha_s(t_s)]}{\Gamma(n + 1 - \alpha_s(t_s)) N^{n-\alpha_s(t_s)} (n - \alpha_s(t_s))} (t_s - a_s)^{n+1-\alpha_s(t_s)}.$$

*Proof* By definition

$${}^C_{a_s} D_{t_s}^{\alpha_s(t_s)}(t^*) = \frac{1}{\Gamma(1 - \alpha_s(t_s))} \int_{a_s}^{t_s} (t_s - \tau)^{-\alpha_s(t_s)} \frac{\partial f}{\partial t_s} [\tau]_s d\tau.$$

In the spirit of [116], we integrate by parts with  $u'(\tau) = (t_s - \tau)^{-\alpha_s(t_s)}$  and  $v(\tau) = \frac{\partial f}{\partial t_s} [\tau]_s$ , and deduce that

$${}^C_{a_s} D_{t_s}^{\alpha_s(t_s)} f(t^*) = \frac{(t_s - a_s)^{1-\alpha_s(t_s)}}{\Gamma(2 - \alpha_s(t_s))} \frac{\partial f}{\partial t_s} [a_s]_s + \frac{1}{\Gamma(2 - \alpha_s(t_s))} \int_{a_s}^{t_s} (t_s - \tau)^{1-\alpha_s(t_s)} \frac{\partial^2 f}{\partial t_s^2} [\tau]_s d\tau.$$

Taking  $u'(\tau) = (t_s - \tau)^{1-\alpha_s(t_s)}$  and  $v(\tau) = \frac{\partial^2 f}{\partial t_s^2} [\tau]_s$ , integrating by parts to obtain

$$\begin{aligned} {}^C_{a_s} D_{t_s}^{\alpha_s(t_s)} f(t^*) &= \frac{(t_s - a_s)^{1-\alpha_s(t_s)}}{\Gamma(2 - \alpha_s(t_s))} \frac{\partial f}{\partial t_s} [a_s]_s + \frac{(t_s - a_s)^{2-\alpha_s(t_s)}}{\Gamma(3 - \alpha_s(t_s))} \frac{\partial^2 f}{\partial t_s^2} [a_s]_s \\ &\quad + \frac{1}{\Gamma(3 - \alpha_s(t_s))} \int_{a_s}^{t_s} (t_s - \tau)^{2-\alpha_s(t_s)} \frac{\partial^3 f}{\partial t_s^3} [\tau]_s d\tau. \end{aligned}$$

By repeating the same process for  $n - 2$  times, we obtain the formula

$$\begin{aligned} {}^C_{a_s} D_{t_s}^{\alpha_s(t_s)} f(t^*) &= \sum_{q=1}^n \frac{(t_s - a_s)^{1-\alpha_s(t_s)}}{\Gamma(q + 1 - \alpha_s(t_s))} \frac{\partial^q f}{\partial t_s^q} [a_s]_s + \frac{1}{\Gamma(n + 1 - \alpha_s(t_s))} \\ &\quad \times \int_{a_s}^{t-s} (t_s - \tau)^{n-\alpha_s(t_s)} \frac{\partial^{n+1} f}{\partial t_s^{n+1}} [\tau]_s d\tau. \end{aligned}$$

Adopting the equalities

$$\begin{aligned} (t_s - \tau)^{n-\alpha_s(t_s)} &= (t_s - a_s)^{n-\alpha_s(t_s)} \left( 1 - \frac{\tau - a_s}{t_s - a_s} \right)^{n-\alpha_s(t_s)} \\ &= (t_s - a_s)^{n-\alpha_s(t_s)} \left[ \sum_{q=0}^N \binom{n - \alpha_s(t_s)}{q} (-1)^q \frac{(\tau - a_s)^q}{(t_s - a_s)^q} + \mathcal{E}^*(t^*) \right] \end{aligned}$$

with

$$\mathcal{E}^*(t^*) = \sum_{q=N+1}^{\infty} \binom{n - \alpha_s(t_s)}{q} (-1)^q \frac{(\tau - a_s)^q}{(t_s - a_s)^q},$$

we obtain

$$\begin{aligned} {}^C_{a_s} D_{t_s}^{\alpha_s(t_s)} f(t^*) &= \sum_{q=1}^n \frac{(t_s - a_s)^{q - \alpha_s(t_s)}}{\Gamma(q + 1 - \alpha_s(t_s))} \frac{\partial^q f}{\partial t_s^q} [a_s]_s + \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \\ &\quad \times \int_{a_s}^{t_s} \sum_{q=0}^N \binom{n - \alpha_s(t_s)}{q} (-1)^q \frac{(\tau - a_s)^q}{(t_s - a_s)^q} \frac{\partial^{n+1}}{\partial t_s^{n+1}} [\tau]_s d\tau + \mathcal{E}(t^*) \\ &= \sum_{q=1}^n \frac{(t_s - a_s)^{q - \alpha_s(t_s)}}{\Gamma(q + 1 - \alpha_s(t_s))} \frac{\partial^q f}{\partial t_s^q} [a_s]_s + \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \\ &\quad \times \sum_{q=0}^N \binom{n - \alpha_s(t_s)}{q} \frac{(-1)^q}{(t_s - a_s)^q} \int_{a_s}^{t_s} (\tau - a_s)^q \frac{\partial^{n+1} f}{\partial t_s^{n+1}} [\tau]_s d\tau + \mathcal{E}(t^*), \end{aligned}$$

where

$$\mathcal{E}(t^*) = \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \int_{a_s}^{t_s} \mathcal{E}^*(t^*) \frac{\partial^{n+1} f}{\partial t_s^{n+1}} [\tau]_s d\tau.$$

Next, we divide the last sum into  $q = 0$  and  $q = 1, 2, \dots, N$  with the notion  $u(\tau) = (\tau - a_s)^q$  and  $v'(\tau) = \frac{\partial^{n+1} f}{\partial t_s^{n+1}} [\tau]_s$ , and use integration by parts technique. Bear in mind that

$$\binom{n - \alpha_s(t_s)}{q} (-1)^q = \frac{\Gamma(\alpha_s(t_s) - n + q)}{\Gamma(\alpha_s(t_s) - n) q!},$$

we get

$$\begin{aligned} &\frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \sum_{q=0}^N \binom{n - \alpha_s(t_s)}{q} \frac{(-1)^q}{(t_s - a_s)^q} \int_{a_s}^{t_s} (\tau - a_s)^q \frac{\partial^{n+1} f}{\partial t_s^{n+1}} [\tau]_s d\tau \\ &= \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \left[ \frac{\partial^n f}{\partial t_s^n} [t_s]_s - \frac{\partial^n f}{\partial t_s^n} [a_s]_s \right] + \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \\ &\quad \times \sum_{q=1}^N \frac{\Gamma(\alpha_s(t_s) - n + q)}{\Gamma(\alpha_s(t_s) - n) q! (t_s - a_s)^q} \left[ (t_s - a_s)^q \frac{\partial^n f}{\partial t_s^n} [t_s]_s - \int_{a_s}^{t_s} q (\tau - a_s)^{q-1} \frac{\partial^n f}{\partial t_s^n} [\tau]_s d\tau \right], \\ &= - \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \frac{\partial^n f}{\partial t_s^n} [a_s]_s + \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \frac{\partial^n f}{\partial t_s^n} [t_s]_s \\ &\quad \times \left[ 1 + \sum_{q=1}^N \frac{\Gamma(\alpha_s(t_s) - n + q)}{\Gamma(\alpha_s(t_s) - n) q!} \right] + \frac{(t_s - a_s)^{n - \alpha_s(t_s) - 1}}{\Gamma(n - \alpha_s(t_s))} \\ &\quad \times \sum_{q=1}^N \frac{\Gamma(\alpha_s(t_s) - n + q)}{\Gamma(\alpha_s(t_s) + 1 - n) (q - 1)! (t_s - a_s)^{q-1}} \int_{a_s}^{t_s} (\tau - a_s)^{q-1} \frac{\partial^n f}{\partial t_s^n} [\tau]_s d\tau. \end{aligned}$$

Therefore, we have

$$\begin{aligned}
{}^C D_{a_s}^{\alpha_s(t_s)} f(t^*) &= \sum_{q=1}^N \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \frac{\partial^n f}{\partial t_s^n} [a_s]_s \\
&+ \frac{(t_s - a_s)^{n - \alpha_s(t_s)}}{\Gamma(n + 1 - \alpha_s(t_s))} \frac{\partial^n f}{\partial t_s^n} [t_s]_s \left[ 1 + \sum_{q=1}^N \frac{\Gamma(\alpha_s(t_s) - n + q)}{\Gamma(\alpha_s(t_s) - n)q!} \right] \\
&+ \frac{(t_s - a_s)^{n - \alpha_s(t_s) - 1}}{\Gamma(n - \alpha_s(t_s))} \sum_{q=1}^N \frac{\Gamma(\alpha_s(t_s) - n + q)}{\Gamma(\alpha_s(t_s) + 1 - n)(q - 1)!(t_s - a_s)^{q-1}} \\
&\times \int_{a_s}^{t_s} (\tau - a_s)^{q-1} \frac{\partial^n f}{\partial t_s^n} [\tau]_s d\tau + \mathcal{E}(t^*).
\end{aligned}$$

By splitting the first term of the last sum and integrate by parts when the procedure is repeated for  $n - 1$  times, we have

$$\begin{aligned}
{}^C D_{a_s}^{\alpha_s(t_s)} f(t^*) &= \\
&\sum_{q=1}^n \frac{(t_s - a_s)^{q - \alpha_s(t_s)}}{\Gamma(q + 1 - \alpha_s(t_s))} \frac{\partial^q f}{\partial t_s^q} [t_s]_s \left[ 1 + \sum_{k=n-q+1}^N \frac{\Gamma(\alpha_s(t_s) - n + k)}{\Gamma(\alpha_s(t_s) - q)(k - n + q)!} \right] \\
&+ \sum_{q=n}^N \frac{\Gamma(\alpha_s(t_s) - n + q)}{\Gamma(1 - \alpha_s(t_s))\Gamma(\alpha_s(t_s))(q - n)!} (t_s - a_s)^{n - q - \alpha_s(t_s)} \\
&\times \int_{a_s}^{t_s} (\tau - a_s)^{q-n} \frac{\partial f}{\partial t_s} [\tau]_s + \mathcal{E}(t^*).
\end{aligned}$$

Using two relations, we seek the upper bound formula for  $\mathcal{E}(t^*)$

$$\left| \frac{\tau - a_s}{t_s - a_s} \right| \leq 1, \quad \text{if } \tau \in [a_s, t_s]$$

and

$$\left| \binom{n - \alpha_s(t_s)}{q} \right| \leq \frac{\exp[(n - \alpha_s(t_s))^2 + n - \alpha_s(t_s)]}{q^{n+1 - \alpha_s(t_s)}},$$

we obtain

$$\begin{aligned}
\mathcal{E}^*(t^*) &\leq \sum_{q=N+1}^{\infty} \frac{\exp[(n - \alpha_s(t_s))^2 + n - \alpha_s(t_s)]}{q^{n+1-\alpha_s(t_s)}} \\
&\leq \int_N^{\infty} \frac{\exp[(n - \alpha_s(t_s))^2 + n - \alpha_s(t_s)]}{q^{n+1-\alpha_s(t_s)}} dq \\
&= \frac{\exp[(n - \alpha_s(t_s))^2 + n - \alpha_s(t_s)]}{N^{n-\alpha_s(t_s)}(n - \alpha_s(t_s))}.
\end{aligned}$$

Then,

$$\mathcal{E}(t^*) \leq M_{n+1}(t^*) \frac{\exp[(n - \alpha_s(t_s))^2 + n - \alpha_s(t_s)]}{\Gamma(n + 1 - \alpha_s(t_s)) N^{n-\alpha_s(t_s)} (n - \alpha_s(t_s))} (t_s - a_s)^{n+1-\alpha_s(t_s)}.$$

The proof is completed.  $\square$

The notions of ordinary and partial fractional operators in relation to both Riemann–Liouville and Caputo integral and derivative of variable fractional-order  $\alpha(t, \tau)$  are introduced.

**Definition 1.6.11** Let  $0 < \alpha(t, \tau) < 1$  for all  $t, \tau \in [a, b]$  and function  $f \in C_1[a, b]$ , with gamma function  $\Gamma$  defined as

$$\Gamma(z) = \int_0^{\infty} e^{-t} t^{z-1} dt.$$

Then,

$${}_a \mathcal{I}_t^{\alpha(t, \tau)} f(t) = \int_a^t \frac{1}{\Gamma(\alpha(t, \tau))} (t - \tau)^{\alpha(t, \tau)-1} f(\tau) d\tau, \quad \text{for } t > a$$

is known as the left Riemann–Liouville fractional integral with variable order  $\alpha(t, \tau)$ , while

$${}_t \mathcal{I}_b^{\alpha(\tau, t)} f(t) = \int_t^b \frac{1}{\Gamma(\alpha(\tau, t))} (t - \tau)^{\alpha(\tau, t)-1} f(\tau) d\tau, \quad \text{for } t < b$$

represents the right Riemann–Liouville fractional integral with variable order  $\alpha(\tau, t)$ .

**Definition 1.6.12** Let  $0 < \alpha(t, \tau) < 1$  for all  $t, \tau \in [a, b]$ . If  ${}_a \mathcal{I}_t^{1-\alpha(t, \tau)} f \in \mathcal{C}[a, b]$ , then the left Riemann–Liouville derivative of fractional variable of order  $\alpha(t, \tau)$  is given by

$${}_a \mathcal{D}_t^{\alpha(t, \tau)} f(t) = \frac{d}{dt} {}_a \mathcal{I}_t^{1-\alpha(t, \tau)} f(t) = \frac{d}{dt} \int_a^t \frac{-1}{\Gamma(1 - \alpha(t, \tau))} (\tau - t)^{-\alpha(t, \tau)} f(\tau) d\tau, \quad \text{for } t > a.$$

Similarly, the right Riemann–Liouville derivative of fractional variable of order  $\alpha(\tau, t)$  is defined by

$${}_t\mathcal{D}_b^{\alpha(\tau,t)} f(t) = -\frac{d}{dt} \mathcal{I}_b^{1-\alpha(\tau,t)} f(t) = \frac{d}{dt} \int_t^b \frac{1}{\Gamma(1-\alpha(\tau,t))} (\tau-t)^{-\alpha(\tau,t)} f(\tau) d\tau, \quad \text{for } t < b.$$

**Definition 1.6.13** Let  $0 < \alpha(t, \tau) < 1$  for all  $t, \tau \in [a, b]$ . If  $f \in \mathcal{C}[a, b]$ , then the left Caputo derivative of fractional variable order  $\alpha(t, \tau)$  is given by

$${}_a^C \mathcal{D}_t^{\alpha(t,\tau)} f(t) = {}_a \mathcal{I}_t^{1-\alpha(t,\tau)} \frac{d}{dt} f(t) = \int_a^t \frac{1}{\Gamma(1-\alpha(t,\tau))} (t-\tau)^{-\alpha(t,\tau)} \frac{d}{d\tau} f(\tau) d\tau \quad \text{for } t > a,$$

while the right Caputo derivative of fractional variable order  $\alpha(\tau, t)$  is defined by

$${}_t^C \mathcal{D}_b^{\alpha(\tau,t)} f(t) = -{}_a \mathcal{I}_t^{1-\alpha(\tau,t)} \frac{d}{dt} f(t) = \int_t^b \frac{1}{\Gamma(1-\alpha(\tau,t))} (t-\tau)^{-\alpha(\tau,t)} \frac{d}{d\tau} f(\tau) d\tau \quad \text{for } t < b.$$

Let  $\Delta_s = [a_1, b_1] \times \cdots \times [a_s, b_s]$ ,  $s \in \mathbb{N}$ , be a subset of  $\mathbb{R}^s$  and  $\mathbf{t} = (t_1, t_2, \dots, t_s) \in \Delta_s$ , and  $\alpha(t, \tau) : [a_i, b_i] \times [a_i, b_i] \rightarrow \mathbb{R}$  be such that  $0 < \alpha_i(t_i, \tau) < 1$  for all  $t_i, \tau \in [a_i, b_i]$ , for  $i = 1, 2, \dots, s$ . Partial derivatives and integrals of fractional variable order are natural generalization which correspond to variable order fractional derivatives and integrals in one dimension.

**Definition 1.6.14** Assume a function  $f = f(t_1, t_2, \dots, t_s)$  is continuous on a set  $\Delta_s$ . The left Riemann–Liouville partial fractional integral with variable order  $\alpha(t, \tau)$ , with respect to the  $i$ th variable  $t_i$ , is defined by

$${}_i \mathcal{I}_{a_i}^{\alpha_i(t_i,\tau)} f(\mathbf{t}) = \int_{a_i}^{t_i} \frac{1}{\Gamma(\alpha_i(t_i,\tau))} (t_i - \tau)^{\alpha_i(t_i,\tau)-1} \times f(t_1, \dots, t_{i-1}, \tau, t_{i+1}, \dots, t_s) d\tau$$

for  $t_i > a_i$ , while

$${}_i \mathcal{I}_{b_i}^{\alpha_i(\tau,t_i)} f(\mathbf{t}) = \int_{t_i}^{b_i} \frac{1}{\Gamma(\alpha_i(\tau,t_i))} (\tau - t_i)^{\alpha_i(\tau,t_i)-1} \times f(t_1, \dots, t_{i-1}, \tau, t_{i+1}, \dots, t_s) d\tau$$

for  $t_i < b_i$ , stands for the right Riemann–Liouville partial fractional integral of variable order  $\alpha_i(\tau, t_i)$ .

**Definition 1.6.15** Given  ${}_i \mathcal{I}_{a_i}^{1-\alpha_i(t_i,\tau)} f \in C^1(\Delta_s)$ , the left Riemann–Liouville partial fractional derivative of variable order  $\alpha_i(t_i, \tau)$ , w.r.t. the  $i$ th variable  $t_i$ , is defined by

$${}_i \mathcal{D}_{a_i}^{\alpha_i(t_i,\tau)} f(\mathbf{t}) = \frac{\partial}{\partial t_i} {}_i \mathcal{I}_{a_i}^{1-\alpha_i(t_i,\tau)} f(\mathbf{t}) = \frac{\partial}{\partial t_i} \int_{a_i}^{t_i} \frac{1}{\Gamma(1-\alpha_i(t_i,\tau))} (t_i - \tau)^{-\alpha_i(t_i,\tau)} \times f(t_1, \dots, t_{i-1}, \tau, t_{i+1}, \dots, t_s) d\tau \quad \text{for } t_i > a_i,$$

and the right Riemann–Liouville partial fractional derivative of variable order  $\alpha_i(\tau, t_i)$ , w.r.t. the  $i$ th variable  $t_i$ , is defined for  $f$  such that  ${}_i \mathcal{I}_{b_i}^{1-\alpha_i(\tau,t_i)} f \in C^1(\Delta_s)$  by

$${}_i D_{b_i}^{\alpha_i(\tau, t_i)} f(\mathbf{t}) = -\frac{\partial}{\partial t_i} {}_i \mathcal{I}_{b_i}^{1-\alpha_i(\tau, t_i)} f(\mathbf{t}) = \frac{\partial}{\partial t_i} \int_{a_i}^{t_i} \frac{-1}{\Gamma(1-\alpha_i(\tau, t_i))} (\tau - t_i)^{-\alpha_i(\tau, t_i)} \\ \times f(t_1, \dots, t_{i-1}, \tau, t_{i+1}, \dots, t_s) d\tau \text{ for } t_i < b_i.$$

**Definition 1.6.16** Let  $f \in C^1(\Delta_s)$ . The left Caputo partial fractional derivative of variable order  $\alpha_i(t_i, \tau)$ , w.r.t. the  $i$ th, variable  $t_i$ , is given by

$${}_i^C D_{a_i}^{\alpha_i(t_i, \tau)} f(\mathbf{t}) = a_i \mathcal{I}_{a_i}^{1-\alpha_i(t_i, \tau)} \frac{\partial}{\partial t_i} f(\mathbf{t}) = \int_{a_i}^{t_i} \frac{1}{\Gamma(1-\alpha_i(t_i, \tau))} (t_i - \tau)^{-\alpha_i(t_i, \tau)} \\ \times \frac{\partial}{\partial \tau} f(t_1, \dots, t_{i-1}, \tau, t_{i+1}, \dots, t_s) d\tau \text{ for } t_i > a_i,$$

while the right Caputo partial fractional derivative of variable order  $\alpha_i(\tau, t_i)$ , w.r.t. the  $i$ th, variable  $t_i$ , is defined by

$${}_i^C D_{b_i}^{\alpha_i(\tau, t_i)} f(\mathbf{t}) = -{}_i \mathcal{I}_{b_i}^{1-\alpha_i(\tau, t_i)} \frac{\partial}{\partial t_i} f(\mathbf{t}) = \int_{t_i}^{b_i} \frac{-1}{\Gamma(1-\alpha_i(\tau, t_i))} (\tau, t_i)^{-\alpha_i(\tau, t_i)} \\ \times \frac{\partial}{\partial \tau} f(t_1, \dots, t_{i-1}, \tau, t_{i+1}, \dots, t_s) d\tau \text{ for } t_i < b_i.$$

*Remark 1.6.17* In Definitions 1.6.14, 1.6.15 and 1.6.16, one observes that all the variables are fixed except  $t_i$ . The choice fixed values helps to determine a function  $f_{t_1, \dots, t_{i-1}, t_{i+1}, \dots, t_s} : [a_i, b_i] \rightarrow \mathbb{R}$  of one variable  $t_i$ ,  $f_{t_1, \dots, t_{i-1}, t_{i+1}, \dots, t_s}(t_i) = f(t_1, \dots, t_{i-1}, \tau, t_{i+1}, \dots, t_s)$ . It should also be noted that partial operators of fractional variable order in the above definitions correspond to partial derivatives and integrals of constant order if  $\alpha_i(\cdot, \cdot)$  is made constant. Details on standard fractional partial operators with constant order can be found in [52, 90, 92, 101, 110].

## 1.7 Tempered Fractional Differentiation

Fractional calculus is known to be a powerful mathematical tool to model most physical phenomena (anomalous diffusion or dispersion), especially where a Lévy motion particle plume in the continuous random walk model moves at a rate irregular with the classical Brownian motion [12]. Fractional integrals and derivatives are convolutions with a power law. When multiplied by an exponential factor results in tempered fractional integrals and derivatives [108]. For instance, the case of a tempered fractional diffusion equation where the partial second derivative term in classical sense is replaced with the tempered fractional derivative, which govern the limits of random walk models with exponentially tempered power-law distribution. The tempered power-law waiting times result in tempered fractional derivatives in time which has been applied and proven useful in geophysics.

Exponentially tempering the Lévy measure is an appropriate means of ensuring that the Lévy flight distributions are finite. Tempered Lévy motions provide a complete set of numerical analysis and statistical physics tools, unlike the truncated

models. Other applications for the tempered fractional derivatives and tempered differential equations can be found, for example, in poroelasticity [42], finance [22, 108], geophysical flows [86] and groundwater hydrology [85, 86]. A reasonable number of numerical methods that are based on finite difference and other high order methods for solving the tempered fractional differential equations have been developed, see [22, 28, 65, 69, 83] and the references therein.

In what follows, we review some existing definitions and properties of tempered fractional differentiation. Let  $[a, b]$  be a finite interval on  $\mathbb{R}$ . We represent  $W([a, b])$  as the integrable space on the finite interval  $[a, b]$ , that is,

$$W([a, b]) = \{w : \|w\|_{W([a, b])} = \int_a^b |w(t)| dt < \infty\}.$$

Also, we let  $AC[a, b]$  be the space of real-valued functions  $w(t)$  and continuous on closed interval  $[a, b]$ . For  $n \in \mathbb{N}^+$ , we let  $C^n[a, b]$  be the space of functions  $w(t)$  that are  $n$  times continuously differentiable on  $[a, b]$ . And let  $AC^n[a, b]$  be real-valued functions  $w(t)$  with continuous derivatives of order  $n - 1$  on interval  $[a, b] : \frac{d^{n-1}}{dx^{n-1}} w(t) \in AC[a, b]$ , that is,

$$AC^n[a, b] = \left\{ w : [a, b] \rightarrow \mathbb{R}, \frac{d^{n-1}}{dx^{n-1}} w(t) \in AC[a, b] \right\}.$$

**Definition 1.7.1** (Riemann–Liouville tempered fractional derivative [12, 22, 65, 101]) For  $n - 1 < \alpha < n$ ,  $n \in \mathbb{N}^+$ ,  $\lambda \geq 0$ . the Riemann–Liouville tempered fractional derivative is given by

$${}_a \mathcal{D}_t^{\alpha, \lambda} w(t) = e^{-\lambda t} {}_a \mathcal{D}_t^\alpha (e^{\lambda t} w(t)) = \frac{e^{-\lambda t}}{\Gamma(n - \alpha)} \frac{d^n}{dt^n} \int_a^t \frac{e^{\lambda \xi} w(\xi)}{(t - \xi)^{\alpha - n + 1}} d\xi, \quad (1.7.1)$$

where  ${}_a \mathcal{D}_t^\alpha (e^{\lambda t} w(t))$  stands for the Riemann–Liouville fractional derivative

$${}_a \mathcal{D}_t^\alpha (e^{\lambda t} w(t)) = \frac{d^n}{dt^n} ({}_a \mathcal{I}_t^{n - \alpha} (e^{\lambda t} w(t))) = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dt^n} \int_a^t \frac{e^{\lambda \xi} w(\xi)}{(t - \xi)^{\alpha - n + 1}} d\xi.$$

*Remark 1.7.2* ([12, 65]) The variants of the Riemann–Liouville tempered fractional derivatives are given as

$${}_a \mathbf{D}_t^{\alpha, t} w(t) = \begin{cases} {}_a \mathcal{D}_t^{\alpha, t} w(t) - \lambda^\alpha w(t), & 0 < \alpha < 1, \\ {}_a \mathcal{D}_t^{\alpha, t} w(t) - \alpha \lambda^{\alpha - 1} \frac{dw(t)}{dt} - \lambda^\alpha w(t), & 1 < \alpha < 2. \end{cases}$$

**Definition 1.7.3** (Riemann–Liouville tempered fractional integral [22, 65]) Assume that the real function  $w(t)$  is piecewise continuous on open interval  $(a, b)$  and  $w(t) \in W([a, b])$ ,  $\rho > 0$ ,  $\lambda \geq 0$ . Then the Riemann–Liouville tempered fractional integral of order  $\rho$  is defined as

$${}_a\mathcal{I}_t^{\rho,\lambda} w(t) = e^{\lambda t} {}_a\mathcal{I}_t^\rho (e^{-\lambda t} w(t)) = \frac{1}{\Gamma(\rho)} \int_a^t e^{-\lambda(t-\xi)} (t-\xi)^{\rho-1} w(\xi) d\xi, \quad (1.7.2)$$

where  ${}_a\mathcal{I}_t^\rho$  is given as the Riemann–Liouville integral

$${}_a\mathcal{I}_t^\rho = \frac{1}{\Gamma(\rho)} \int_a^t (t-\xi)^{\rho-1} w(\xi) d\xi.$$

Clearly, we can see that when  $\lambda = 1$ , the tempered fractional integral (1.7.2) reduces to the standard Riemann–Liouville fractional integral. In some practical applications, the fractional integral is sometimes represented as  ${}_a\mathcal{D}^{-\rho,\lambda} w(t)$ .

**Definition 1.7.4** (Riemann–Liouville fractional substantial derivative [34, 117]) For  $n-1 < \alpha < n$ ,  $n \in \mathbb{N}^+$ , and let  $\lambda(x)$  be any given function in the spatial domain. the Riemann–Liouville fractional substantial derivative is expressed by

$$\mathcal{D}_s^{\alpha,\lambda(x)} w(t) = \left( \frac{d}{dt} + \lambda(x) \right)^n {}_a\mathcal{I}_t^{n-\alpha,\lambda(x)} w(t) = \left( \frac{d}{dt} + \lambda(x) \right)^n \int_a^t \frac{e^{-\lambda(x)\cdot(t-\xi)}}{(t-\xi)^{\alpha-n+1}} w(\xi) d\xi, \quad (1.7.3)$$

where  ${}_a\mathcal{I}_t^{n-\alpha,\lambda(x)}$  represents the Riemann–Liouville fractional integral and

$$\left( \frac{d}{dt} + \lambda(x) \right)^n = \underbrace{\left( \frac{d}{dt} + \lambda(x) \right) \cdots \left( \frac{d}{dt} + \lambda(x) \right)}_{n \text{ times}}.$$

*Remark 1.7.5* The Riemann–Liouville fractional substantial derivative (1.7.3) is equivalent to the Riemann–Liouville tempered fractional derivative (1.7.1) if the given function  $\lambda(x)$  is nonnegative. By adapting integration by parts technique, we have

$$\begin{aligned} & \left( \frac{d}{dt} + \lambda(x) \right)^n \left[ \int_a^t e^{-\lambda(t-\xi)} (t-\xi)^{\rho-1} w(\xi) d\xi \right] \\ &= \left( \frac{d}{dt} + \lambda(x) \right)^{n-1} \left[ \left( \frac{d}{dt} + \lambda(x) \right) \int_a^t \frac{e^{-\lambda(x)\cdot(t-\xi)}}{(t-\xi)^{\alpha-n+1}} w(\xi) d\xi \right] \\ &= \left( \frac{d}{dt} + \lambda(x) \right)^{n-1} \left[ e^{-\lambda(x)t} \frac{d}{dt} \int_a^t \frac{e^{\lambda(x)\xi}}{(t-\xi)^{\alpha-n+1}} w(\xi) d\xi \right] \\ &= \left( \frac{d}{dt} + \lambda(x) \right)^{n-2} \left[ e^{-\lambda(x)t} \frac{d^2}{dt^2} \int_a^t \frac{e^{\lambda(x)\xi}}{(t-\xi)^{\alpha-n+1}} w(\xi) d\xi \right] \\ &= \dots \\ &= {}_a\mathcal{D}^{\alpha,\lambda(x)} w(t). \end{aligned}$$

The tempered  $n$ -th order derivative of  $w(t)$  is equivalent to  $\left( \frac{d}{dt} + \lambda \right)^n w(t)$ , which for simplicity is denoted as  $\mathcal{D}^{n,\lambda} w(t)$ .

**Definition 1.7.6** (Caputo tempered fractional derivative [110, 115]) For  $n - 1 < \alpha < n$ ,  $n \in \mathbb{N}^+$ ,  $\lambda \geq 0$ . The Caputo tempered fractional derivative is an expression of the form

$${}^C_a\mathcal{D}_t^{\alpha,\lambda}w(t) = e^{-\lambda t} {}^C_a\mathcal{D}_t^\alpha(e^{\lambda t}w(t)) = \frac{e^{-\lambda t}}{\Gamma(n-\alpha)} \int_a^t \frac{1}{(t-\xi)} \frac{d^n(e^{\lambda\xi})}{d\xi^n} w(\xi) d\xi, \quad (1.7.4)$$

where  ${}^C_a\mathcal{D}_t^{\alpha,\lambda}(e^{\lambda t}w(t))$  represents the Caputo fractional derivative [101]

$${}^C_a\mathcal{D}_t^{\alpha,\lambda}(e^{\lambda t}w(t)) = \frac{1}{\Gamma(n-\alpha)} \int_a^t \frac{1}{(t-\xi)} \frac{d^n(e^{\lambda\xi})}{d\xi^n} w(\xi) d\xi.$$

*Remark 1.7.7* The Riemann–Liouville tempered fractional derivative (1.7.1) is equivalent to the Caputo tempered fractional derivative (1.7.4) if  ${}_a\mathcal{D}_t^{\alpha,\lambda}w(t) = \mathcal{D}^{n,\lambda} {}_a\mathcal{I}_t^{n-\alpha,\lambda}w(t)$  and  ${}^C_a\mathcal{D}_t^{\alpha,\lambda}w(t) = {}_a\mathcal{I}_t^{n-\alpha,\lambda}\mathcal{D}^{n-\alpha,\lambda}w(t)$ , respectively.

It should also be noted that when  $\lambda = 0$ , the Riemann–Liouville or Caputo tempered fractional derivatives reduce to the Riemann–Liouville or Caputo fractional derivatives.

**Proposition 1.7.8** (Composite properties)

1. Let  $w(x) \in W([a, b])$  and  $\mathcal{I}^{n-\alpha,\lambda}w(t) \in AC^n[a, b]$ . Then the Riemann–Liouville tempered fractional derivative and fractional integral have all composite properties

$${}_a\mathcal{I}_t^{\alpha,\lambda} [{}_a\mathcal{D}_t^{\alpha,\lambda}w(t)] = w(t) - \sum_{j=0}^{n-1} \frac{e^{-\lambda t}(t-a)^{\alpha-j-1}}{\Gamma(\alpha-j)} [{}_a\mathcal{D}_t^{\alpha-j-1}(e^{\lambda t}w(t))|_{t=a}], \quad (1.7.5)$$

and

$${}_a\mathcal{D}_t^{\alpha,\lambda} [{}_a\mathcal{I}_t^{\alpha,\lambda}w(t)] = w(t). \quad (1.7.6)$$

2. Let  $w(t) \in AC^n[a, b]$  and  $n - 1 < \alpha < n$ . Then the Riemann–Liouville tempered fractional integral and the Caputo fractional derivative have the composite properties

$${}_a\mathcal{I}_t^{\alpha,\lambda} [{}^C_a\mathcal{D}_t^{\alpha,\lambda}w(t)] = w(t) - \sum_{j=0}^{n-1} e^{-\lambda t} \frac{(t-a)^j}{j!} \left[ \frac{d^j(e^{\lambda t}w(t))}{dt^j} \Big|_{t=a} \right], \quad (1.7.7)$$

and

$${}^C_a\mathcal{D}_t^{\alpha,\lambda} [{}_a\mathcal{I}_t^{\alpha,\lambda}w(t)] = w(t) \quad \text{if } \alpha \in (0, 1). \quad (1.7.8)$$

*Proof* We recall from the definition of the Riemann–Liouville tempered fractional derivative and integral that

$$\begin{aligned}
{}_a\mathcal{I}_t^{\alpha,\lambda} [{}_a\mathcal{D}_t^{\alpha,\lambda} w(t)] &= e^{-\lambda t} {}_a\mathcal{I}_t^\alpha [e^{\lambda t} ({}_a\mathcal{D}_t^{\alpha,\lambda} w(t))] \\
&= e^{-\lambda t} {}_a\mathcal{I}_t^\alpha [e^{\lambda t} (e^{-\lambda t} {}_a\mathcal{D}_t^\alpha (e^{\lambda t} w(t)))] \\
&= e^{-\lambda t} \underbrace{{}_a\mathcal{I}_t^\alpha [{}_a\mathcal{D}_t^\alpha (e^{\lambda t} w(t))]}_{(\mathcal{I})}.
\end{aligned} \tag{1.7.9}$$

Using the composition formula [68, 101]

$${}_a\mathcal{I}_t^\alpha [{}_a\mathcal{D}_t^\alpha u(t)] = u(t) - \sum_{j=0}^{n-1} \frac{(t-a)^{\alpha-j-1}}{\Gamma(\alpha-j)} [{}_a\mathcal{D}_t^{\alpha-j-1} (u(t))|_{t=a}],$$

we obtain

$$(\mathcal{I}) = {}_a\mathcal{I}_t^\alpha [{}_a\mathcal{D}_t^\alpha e^{\lambda t} w(t)] = e^{\lambda t} w(t) - \sum_{j=0}^{n-1} \frac{(t-a)^{\alpha-j-1}}{\Gamma(\alpha-j)} [{}_a\mathcal{D}_t^{\alpha-j-1} (e^{\lambda t} w(t))|_{t=a}].$$

By substituting the above into (1.7.9) we recover (1.7.5). From the Riemann–Liouville tempered fractional derivative and integral definitions, there exists

$$\begin{aligned}
{}_a\mathcal{D}_t^{\alpha,\lambda} [{}_a\mathcal{I}_t^{\alpha,\lambda} w(t)] &= e^{-\lambda t} {}_a\mathcal{D}_t^\alpha [e^{\lambda t} ({}_a\mathcal{I}_t^{\alpha,\lambda} w(t))] \\
&= e^{-\lambda t} {}_a\mathcal{D}_t^\alpha [e^{\lambda t} (e^{-\lambda t} {}_a\mathcal{I}_t^\alpha (e^{\lambda t} w(t)))] \\
&= e^{-\lambda t} {}_a\mathcal{D}_t^\alpha [{}_a\mathcal{I}_t^\alpha (e^{\lambda t} w(t))].
\end{aligned}$$

By using the composite properties of Riemann–Liouville fractional derivative and integral [65, 68, 110]

$${}_a\mathcal{D}_t^\alpha [{}_a\mathcal{I}_t^\alpha (u(t))] = u(t) \tag{1.7.10}$$

by putting  $u(t) = e^{\lambda t} w(t)$  in (1.7.10), we have

$${}_a\mathcal{D}_t^{\alpha,\lambda} [{}_a\mathcal{I}_t^{\alpha,\lambda} w(t)] = e^{-\lambda t} {}_a\mathcal{D}_t^\alpha [{}_a\mathcal{I}_t^\alpha (e^{\lambda t} w(t))] = w(t).$$

In a similar way, we use the composite properties of Caputo derivative [68, 101, 110]

$${}_a\mathcal{I}_t^\alpha [{}_a^C\mathcal{D}_t^\alpha u(t)] = u(t) - \sum_{j=0}^{n-1} \frac{(t-a)^j}{j!} \left[ \frac{d^j u(t)}{dt^j} \Big|_{t=a} \right],$$

and

$${}_a^C\mathcal{D}_t^\alpha [{}_a\mathcal{I}_t^\alpha (u(t))] = u(t), \quad \text{if } \alpha \in (0, 1).$$

Following a similar process, we can get (1.7.7) and (1.7.8).  $\square$

### 1.7.1 Properties of Tempered Fractional Derivative and Integral

We have the following properties for the Riemann–Liouville tempered fractional integral.

**Lemma 1.7.9** *If  $w(t) \in AC^n[a, b]$ ,  $\rho > 0$  and  $\lambda \in \mathbb{R}$ , then for all  $t \geq a$ ,*

$$\begin{aligned} {}_a\mathcal{I}_t^{\rho, \lambda} w(t) &= \sum_{j=1}^n \frac{e^{-\lambda t} (t-a)^{\rho+j-1}}{\Gamma(\rho+j)} \left[ \frac{d^{j-1}(e^{\lambda t} w(t))}{dt^{j-1}} \Big|_{t=a} \right] \\ &\quad + \frac{e^{-\lambda t}}{\Gamma(\rho+n)} \int_0^t (t-\xi)^{\rho+n-1} \frac{d^n}{d\xi^n} (e^{\lambda \xi} w(\xi)) d\xi. \end{aligned}$$

*Proof* If  $w(t)$  is continuous for  $t \geq a$ , then apply integration by parts to (1.7.1), there exists

$$\frac{1}{\Gamma(\rho)} \int_a^t (t-\xi)^{\rho-1} e^{\lambda \xi} w(\xi) d\xi = \frac{(t-a)^\rho w(a)}{\Gamma(\rho+1)} + \frac{1}{\Gamma(\rho+1)} \int_a^t (t-\xi)^\rho \frac{d}{d\xi} e^{\lambda \xi} w(\xi) d\xi,$$

and if the given function is  $n$  continuous derivatives, we integrate by parts to obtain

$$\begin{aligned} \frac{1}{\Gamma(\rho)} \int_a^t (t-\xi)^{\rho-1} e^{\lambda \xi} w(\xi) d\xi &= \sum_{j=1}^n \frac{(t-a)^{\rho+j-1}}{\Gamma(\rho+j)} \left[ \frac{d^{j-1}(e^{\lambda t} w(t))}{dt^{j-1}} \Big|_{t=a} \right] \\ &\quad + \frac{1}{\Gamma(\rho+n)} \int_0^t (t-\xi)^{\rho+n-1} \frac{d^n}{d\xi^n} (e^{\lambda \xi} w(\xi)) d\xi. \end{aligned} \tag{1.7.11}$$

The desired result is achieved when we multiply both sides of (1.7.11) by function  $e^{-\lambda t}$ .  $\square$

In addition, integrating by parts results in

$${}_a\mathcal{I}_t^{\rho, \lambda} w(t) = e^{\rho t} w(a) + \rho \int_a^t e^{-\rho(t-\xi)} w(\xi) d\xi + \int_a^t e^{-r h \rho(x-\xi)} dw(\xi),$$

which indicates that if  $w(t)$  has continuous derivatives on the finite domain  $[a, b]$ , and  $\rho > 0$ , then for all  $t \geq a$ ,

$$\lim_{\rho \rightarrow 0} {}_a\mathcal{I}_t^{\rho, \lambda} w(t) = w(t).$$

**Proposition 1.7.10** For a function  $w(t) \in W([a, b])$ ,  $\rho > 0$ ,  $\lambda \in \mathbb{R}$ , we have

$$\left\| \frac{1}{\Gamma(\rho)} \int_a^t e^{-\lambda(t-\xi)} (t-\xi)^{\rho-1} w(\xi) d\xi \right\|_{W([a,b])} \leq G \|w\|_{W([a,b])},$$

where  $G = \frac{(b-a)^\rho}{\Gamma(\rho+1)}$ .

*Proof* By calculation, we get

$$\begin{aligned} & \left\| \frac{1}{\Gamma(\rho)} \int_a^t e^{-\lambda(t-\xi)} (t-\xi)^{\rho-1} w(\xi) d\xi \right\|_{W([a,b])} \\ & \leq \frac{1}{\Gamma(\rho)} \int_a^b \int_a^t e^{-\lambda(t-\xi)} (t-\xi)^{\rho-1} |u(\xi)| d\xi dt \\ & \leq \frac{1}{\Gamma(\rho)} \int_a^b \int_\xi^b e^{-\lambda(t-\xi)} (t-\xi)^{\rho-1} dt |w(\xi)| d\xi \\ & \leq \frac{(b-a)^\rho}{\Gamma(\rho+1)} \|w\|_{W([a,b])}. \end{aligned}$$

□

**Proposition 1.7.11** (Linearity properties) Let  $w(t) \in W([a, b])$ . Then for all  $\sigma, \tau, \lambda \in \mathbb{R}$ :

1. for  $\sigma > 0$ , satisfies

$${}_a \mathcal{I}_t^{\rho, \lambda} [\sigma w(t) + \tau w(t)] = \sigma {}_a \mathcal{I}_t^{\rho, \lambda} [w(t)] + \tau {}_a \mathcal{I}_t^{\rho, \lambda} [w(t)],$$

2. for  $\alpha \in (n-1, n)$ , satisfies

$${}_a \mathcal{D}_t^{\alpha, \lambda} [\sigma w(t) + \tau w(t)] = \sigma {}_a \mathcal{D}_t^{\alpha, \lambda} [w(t)] + \tau {}_a \mathcal{D}_t^{\alpha, \lambda} [w(t)],$$

3. for  $\alpha \in (n-1, n)$ , satisfies

$${}_a^C \mathcal{D}_t^{\alpha, \lambda} [\sigma w(t) + \tau w(t)] = \sigma {}_a^C \mathcal{D}_t^{\alpha, \lambda} [w(t)] + \tau {}_a^C \mathcal{D}_t^{\alpha, \lambda} [w(t)].$$

*Proof* Details of this proof are omitted here. The linearity of fractional derivatives and integral is directly followed from the corresponding definitions. □

**Proposition 1.7.12** (Semi-group property) Let  $w(t) \in W([a, b])$  and  $\rho_1, \rho_2 > 0$ ,  $\lambda \in \mathbb{R}$ . Then for all  $t \geq a$ ,

$${}_a \mathcal{I}_t^{\rho_1, \lambda} [{}_a \mathcal{I}_t^{\rho_2, \lambda}] = {}_a \mathcal{I}_t^{\rho_1 + \rho_2, \lambda} w(t) = {}_a \mathcal{I}_t^{\rho_2, \lambda} [{}_a \mathcal{I}_t^{\rho_1, \lambda} w(t)].$$

*Proof* With reference to the semi-group property of Riemann–Liouville fractional integral (see, Podlubny [101])  $\mathcal{I}_t^{\rho_1} \mathcal{I}_t^{\rho_2} w(t) = \mathcal{I}_t^{\rho_1 + \rho_2} w(t)$ , we obtain the following tempered semi-group property of fractional integral

$$\begin{aligned} {}_a \mathcal{I}_t^{\rho_1, \lambda} [{}_a \mathcal{I}_t^{\rho_2, \lambda} w(t)] &= e^{-\lambda t} {}_a \mathcal{I}_t^{\rho_1} [e^{\lambda t} ({}_a \mathcal{I}_t^{\rho_2, \lambda} w(t))] \\ &= e^{-\lambda t} {}_a \mathcal{I}_t^{\rho_1} [e^{\lambda t} (e^{-\lambda t} a \mathcal{I}_t^{\rho_2, \lambda} (e^{\lambda t} w(t)))] \\ &= e^{-\lambda t} {}_a \mathcal{I}_t^{\rho_1} [a \mathcal{I}_t^{\rho_2} (e^{\lambda t} w(t))] \\ &= e^{-\lambda t} {}_a \mathcal{I}_t^{\rho_1 + \rho_2} (e^{\lambda t} w(t)) \\ &= a \mathcal{I}_t^{\rho_1 + \rho_2, \lambda} w(t). \end{aligned}$$

□

The tempered fractional calculus is a linear operation, similar to fractional calculus.

**Proposition 1.7.13** *Let  $w(t) \in C^n[a, b]$  and  $\alpha \in (n - 1, n)$ . Then for all  $t \in [a, b]$ , there exists*

$${}_a^C \mathcal{D}_t^{\alpha, \lambda} [w(t)]|_{t=a} = 0.$$

*Proof* With simple argument, we obtain

$$\left| {}_a^C \mathcal{D}_t^{\alpha, \lambda} \right| \leq \left| \frac{e^{-\lambda t}}{\Gamma(n - \alpha)} \int_a^t \frac{1}{(t - \xi)^{\alpha - n + 1}} \frac{d^n e^{\lambda \xi} w(\xi)}{d\xi^n} d\xi \right| \leq \frac{G e^{-\lambda t} (t - a)^{n - \alpha}}{\Gamma(n - \alpha + 1)},$$

where  $G = \max_{t \in [a, b]} \left| \frac{d^n e^{\lambda t} w(t)}{dt^n} \right|$ . Hence, we obtain the desired result from the above analysis. □

## 1.7.2 Laplace Transforms of the Tempered Fractional Calculus

Recall that the Laplace transform of a function, say  $f(t)$  and its inverse are, respectively, defined as [111]

$$\mathcal{L}\{f(t); s\} = \bar{f}(s) = \int_0^{+\infty} e^{-st} f(t) dt,$$

and

$$\mathcal{L}^{-1}\{\bar{f}(s); t\} = f(t) = \frac{1}{2\pi i} \int_{s_0 - i\infty}^{s_0 + i\infty} e^{st} \bar{f}(s) ds, \quad s_0 = \operatorname{Re}(s) > 0, \quad i^2 = -1.$$

We begin with the Laplace transform of the Riemann–Liouville tempered fractional integral with order  $\rho$ .

**Proposition 1.7.14** *The Laplace transform of the Riemann–Liouville tempered fractional integral is defined as*

$$\mathcal{L}\left({}_0\mathcal{I}_t^{\rho,\lambda} f(t)\right) = (\lambda + s)^{-\rho} \bar{f}(s).$$

*Proof* In the form of convolution, we first rewrite the Riemann–Liouville tempered fractional integral

$${}_0\mathcal{I}_t^{\rho,\lambda} f(t) = \frac{1}{\Gamma(\rho)} \int_0^t e^{-\lambda(t-s)} (t-s)^{\rho-1} f(s) ds = \frac{e^{-\lambda t} t^{\rho-1}}{\Gamma(\rho)} \bullet f(t).$$

With reference to the Laplace convolution in [111]

$$\mathcal{L}\{f(t) \bullet u(t); s\} = \bar{f}(s) \bar{u}(s),$$

we obtain

$$\mathcal{L}\{{}_0\mathcal{I}_t^{\rho,\lambda} f(t); s\} = \mathcal{L}\left\{\frac{e^{-\lambda t} t^{\rho-1}}{\Gamma(\rho)}; s\right\} \mathcal{L}\{f(t); s\}.$$

Recall that the Laplace transform

$$\mathcal{L}\{e^{-\lambda t} t^{\rho-1}; s\} = \Gamma(\rho)(\lambda + s)^{-\rho},$$

we get the Laplace transform of Riemann–Liouville tempered fractional integral

$$\mathcal{L}\left\{{}_0\mathcal{I}_t^{\rho,\lambda} f(t); s\right\} = (\lambda + s)^{-\rho} \bar{f}(s).$$

□

Next, we consider the Laplace transform of tempered fractional for the Riemann–Liouville and the Caputo derivatives.

**Proposition 1.7.15** *The Laplace transform of the Riemann–Liouville tempered fractional derivative is defined by*

$$\mathcal{L}\{{}_0\mathcal{D}_t^{\alpha,\lambda} f(t); s\} = (s + \lambda)^\alpha \bar{f}(s) - \sum_{j=0}^{n-1} (s + \lambda)^j \left[ {}_0\mathcal{D}_t^{\alpha-j-1} (e^{\lambda t} f(t)) \right] \Big|_{t=0} \quad (1.7.12)$$

and the Laplace transform of the Caputo tempered fractional derivative is defined as

$$\mathcal{L}\{{}_0^C\mathcal{D}_t^{\alpha,\lambda} f(t); s\} = (s + \lambda)^\alpha \bar{f}(s) - \sum_{j=0}^{n-1} (s + \lambda)^{\alpha-j-1} \left[ \frac{d^j}{dt^j} (e^{\lambda t} f(t)) \right] \Big|_{t=0}. \quad (1.7.13)$$

*Proof* Considering the Riemann–Liouville tempered fractional calculus properties, we can write the Riemann–Liouville tempered fractional derivative as

$${}_0\mathcal{D}_t^{\alpha,\lambda} f(t) = e^{-\lambda t} \frac{d^n}{dt^n} (u(t)), \quad n-1 < \alpha < n,$$

where  $u(t)$  is denoted by

$$u(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t \frac{e^{\lambda s} f(s)}{(t-s)^{\alpha-n+1}} ds = {}_0\mathcal{I}_t^{n-\alpha} (e^{\lambda t} f(t)).$$

Further, we use the Laplace transform with integer-order derivative formula

$$\begin{aligned} \mathcal{L} \left\{ \frac{d^n}{dt^n} u(t); s \right\} &= s^n \bar{u}(s) - \sum_{j=0}^{n-1} s^{n-j-1} \left[ \frac{d^j}{dt^j} u(t) \right] \Big|_{t=0} \\ &= s^n \bar{u}(s) - \sum_{j=0}^{n-1} s^j \left[ \frac{d^{n-j-1}}{dt^{n-j-1}} u(t) \right] \Big|_{t=0}. \end{aligned}$$

From the first translation Theorem [65, 111]

$$\mathcal{L}\{e^{-\lambda t} f(t); s\} = \bar{f}(\lambda + s), \quad \lambda \in \mathbb{R}, \quad \operatorname{Re}(s) > \lambda, \quad (1.7.14)$$

we obtain

$$\mathcal{L} \left\{ e^{6-\lambda t} \frac{d^n}{dt^n} u(t); s \right\} = (s + \lambda)^n \bar{u}(s + \lambda) - \sum_{j=0}^{n-1} (s + \lambda)^j \left[ \frac{d^{n-j-1}}{dt^{n-j-1}} u(t) \right] \Big|_{t=0},$$

which shows that

$$\mathcal{L}\{{}_0\mathcal{D}_t^{\alpha,\lambda} f(t); s\} = (s + \lambda)^n \bar{u}(s + \lambda) - \sum_{j=0}^{n-1} (s + \lambda)^j \left[ \frac{d^{n-j-1}}{dt^{n-j-1}} u(t) \right] \Big|_{t=0}. \quad (1.7.15)$$

Applying the convolution theorem once more leads to

$$\begin{aligned} \mathcal{L}\{u(t); s\} &= \mathcal{L}\{{}_0\mathcal{I}_t^{n-\alpha} (e^{\lambda t} f(t))\} \\ &= \mathcal{L} \left\{ \frac{t^{n-\alpha-1}}{\Gamma(n-\alpha)}; s \right\} \mathcal{L}\{(e^{\lambda t} f(t));\} \\ &= s^{-(n-\alpha)} \bar{f}(s - \lambda). \end{aligned}$$

On combining the above formulae, we get

$$\bar{u}(s + \lambda) = (s + \lambda)^{-(n-\alpha)} \bar{f}(s). \quad (1.7.16)$$

It follows directly from the definition of the Riemann–Liouville fractional integral that

$$\frac{d^{n-j-1}}{dt^{n-j-1}}u(t) = \frac{d^{n-j-1}}{dt^{n-j-1}} \mathcal{I}_t^{n-\alpha}(e^{\lambda t} f(t)) = {}_0\mathcal{D}_t^{-(j-\alpha+1)}(e^{\lambda t} f(t)). \quad (1.7.17)$$

Putting Eqs. (1.7.16) and (1.7.17) into (1.7.17), we obtain

$$\mathcal{L}\{{}_0\mathcal{D}_t^{\alpha,\lambda} f(t); s\} = (s + \lambda)^\alpha \bar{f}(s) - \sum_{j=0}^{n-1} (s + \lambda)^j {}_0\mathcal{D}_t^{-(j-\alpha+1)}(e^{\lambda t} f(t))|_{t=0}.$$

In Caputo sense, the Laplace transform for the tempered fractional derivative can be written as

$$\begin{aligned} {}_0^C\mathcal{D}_t^{\alpha,\lambda} f(t) &= e^{-\lambda t} {}_0^C\mathcal{D}_t^\alpha(e^{\lambda t} f(t)) = e^{-\lambda t} {}_0\mathcal{I}_t^{n-\alpha}(u(t)), \\ u(t) &= \frac{d^n}{dt^n}(v(t)), \\ v(t) &= e^{\lambda t} f(t). \end{aligned}$$

Adapting the first translation theorem and the Riemann–Liouville fractional integral (1.7.14) [111], we have

$$\mathcal{L}\{{}_0^C\mathcal{D}_t^{\alpha,\lambda} f(t); s\} = (s + \lambda)^{-(n-\alpha)} \bar{u}(s + \lambda), \quad (1.7.18)$$

where

$$\bar{u}(s + \lambda) = (s + \lambda)^n \bar{v}(s + \lambda) - \sum_{j=0}^{s-1} (s + \lambda)^{\alpha-j-1} \left[ \frac{d^j}{dt^j} v(t) \right] \Big|_{t=0}.$$

Bear in mind that  $\mathcal{L}\{v(t); s\} = \bar{f}(s - \lambda)$ , and putting the above formula into (1.7.18), we recall the Laplace transform of the Caputo tempered fractional derivative (1.7.13).  $\square$

*Remark 1.7.16* With  $\lambda = 0$  in Eq. (1.7.12), one easily obtains the Laplace transform of the Riemann–Liouville fractional derivative [101]

$$\mathcal{L}\{{}_0\mathcal{D}_t^\alpha f(t); s\} = s^\alpha \bar{f}(s) - \sum_{j=0}^{n-1} s^j \left[ {}_0\mathcal{D}_t^{-(j-\alpha+1)}(f(t))|_{t=0} \right].$$

Similarly, if  $\lambda = 0$  in (1.7.13), we obtain the Laplace transform of Caputo derivative [101]

$$\mathcal{L}\{ {}_0^C \mathcal{D}_t^\alpha f(t); s \} = s^\alpha \bar{f}(s) - \sum_{j=0}^{n-1} s^{\alpha-j-1} \left[ \frac{d^j f(t)}{dt^j} \Big|_{t=0} \right], \quad n-1 < \alpha < n.$$

Observation from the Laplace transform of tempered fractional derivatives shows that different initial value conditions are required for fractional differential equations with different fractional derivatives. It should also be noted from Eq. (1.7.13) that the Laplace transform for the Caputo tempered fractional derivative requires the values of the function  $f(t)$  and its derivatives at  $t = 0$ , which are specified in physical. So the Caputo type fractional derivatives are often applied in time direction, see, for instance, [7, 8, 11, 13, 20, 21, 101] and the references therein.

## 1.8 Caputo–Fabrizio Fractional Differentiation

One of the most recent fractional derivative that was proposed in literature is the Caputo–Fabrizio fractional derivative [8, 20, 75]. It was mentioned in their research papers that the new derivative possess additional motivating properties than the previously existing versions. The fractional derivative proposed in [20] with a smooth kernel based on two different representation for the spatial variable and time. The first definition performs better on the time variables; which make it easier and suitable to use the Laplace transform. The second definition is related to the spatial variables, by a non-local fractional derivative, for which it is more convenient to use with the Fourier transform.

Here we start by presenting the definition of the known Caputo fractional derivative of order  $\alpha$  with  $\alpha \in [0, 1]$  and  $a \in [-\infty, t)$ ,  $f \in H^1(a, b)$ ,  $b > a$ , defined by [18, 52, 75]

$${}^C \mathcal{D}_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_a^t \frac{f(s)}{(t-s)^\alpha} ds. \quad (1.8.1)$$

By changing the kernel  $(t-s)^{-\alpha}$  with the function  $\exp\left(-\frac{\alpha}{1-\alpha}t\right)$  and  $\frac{1}{\Gamma(1-\alpha)}$  with  $\frac{M(\alpha)}{1-\alpha}$  one gets the Caputo–Fabrizio fractional derivative of order  $0 < \alpha < 1$  as introduced in [20]. That is,

$${}^{CF} \mathcal{D}_t^\alpha f(t) = \frac{M(\alpha)}{(1-\alpha)} \int_a^t f(s) \exp\left[-\frac{\alpha(t-s)}{1-\alpha}\right] ds, \quad (1.8.2)$$

where  $M(\alpha)$  is known to be a normalized function such that  $M(0) = M(1) = 1$ . According to their definition, if  $f$  is a constant function, then  ${}^{CF} \mathcal{D}_t^\alpha f = 0$ , as in the case of elderly Caputo fractional derivative. The major difference between the Caputo and the Caputo–Fabrizio definition is that, contrary to the formal definition, the new kernel possesses no singularity for  $t = s$ .

### 1.8.1 Caputo–Fabrizio Fractional Derivative in Caputo Sense

In [20], the proposed derivative was also applied to functions that do not belong to  $H^1(a, b)$ . The definition in (1.8.2) was formulated for  $f \in W^1(-\infty, b)$ , for any  $\alpha \in [0, 1]$  as

$${}^{CF}\mathcal{D}_t^\alpha f(t) = \frac{\alpha M(\alpha)}{(1-\alpha)} \int_{-\infty}^t (f(t) - f(s)) \exp\left[-\frac{\alpha(t-s)}{1-\alpha}\right] ds.$$

By putting

$$\gamma = \frac{1-\alpha}{\alpha} \in [0, \infty], \quad \alpha = \frac{1}{1+\gamma} \in [0, 1]$$

the definition (1.8.2) takes the form

$${}^{CF}\mathbf{D}_t^\gamma = \frac{N(\gamma)}{\gamma} \int_a^t \dot{f}(s) \exp\left[-\frac{(t-s)}{\gamma}\right] ds, \quad (1.8.3)$$

where  $\gamma \in [0, \infty]$  and  $N(\gamma)$  is the normalization constant that corresponds to  $M(\alpha)$ , in such that  $N(0) = N(\infty) = 1$ . Since

$$\lim_{\gamma \rightarrow 0} \frac{1}{\gamma} \exp\left[-\frac{(t-s)}{\gamma}\right] = \sigma(t-s)$$

and for  $\alpha \rightarrow 1$ , we have  $\gamma \rightarrow 0$ . Then

$$\begin{aligned} \lim_{\alpha \rightarrow 1} {}^{CF}\mathcal{D}_t^\alpha f(t) &= \lim_{\alpha \rightarrow 1} \frac{M(\alpha)}{1-\alpha} \int_a^t \dot{f}(s) \exp\left[-\frac{\alpha(t-s)}{1-\alpha}\right] ds \\ &= \lim_{\gamma \rightarrow 0} \frac{N(\gamma)}{\gamma} \int_a^t \dot{f}(s) \exp\left[-\frac{(t-s)}{\gamma}\right] ds = \dot{f}(t). \end{aligned} \quad (1.8.4)$$

But if  $\alpha \rightarrow 0$ , when  $\gamma \rightarrow +\infty$ , then

$$\begin{aligned} \lim_{\alpha \rightarrow 0} {}^{CF}\mathcal{D}_t^\alpha f(t) &= \lim_{\alpha \rightarrow 0} \frac{M(\alpha)}{1-\alpha} \int_a^t \dot{f}(s) \exp\left[-\frac{\alpha(t-s)}{1-\alpha}\right] ds \\ &= \lim_{\gamma \rightarrow +\infty} \frac{N(\gamma)}{\gamma} \int_a^t \dot{f}(s) \exp\left[-\frac{(t-s)}{\gamma}\right] ds = f(t) - f(a). \end{aligned} \quad (1.8.5)$$

### 1.8.2 The Laplace Transform of the Caputo–Fabrizio Fractional Derivative

It is well established that Laplace Transform plays an important role in the study of ordinary differential equations. In order to study the properties of the Caputo–Fabrizio fractional derivative as given in Eq. (1.8.3) with  $a = 0$  and variable  $\tau$  as

$$\mathcal{L} [{}^{CF}\mathcal{D}_t^\alpha f(t)] = \frac{1}{(1-\alpha)} \int_0^\infty \exp -\tau t \int_0^t \dot{f}(s) \exp -\frac{\alpha(t-s)}{1-\alpha} ds dt.$$

By using the convolution property, we obtain

$$\mathcal{L} [{}^{CF}\mathcal{D}_t^\alpha f(t)] = \frac{1}{(1-\alpha)} \mathcal{L}(\dot{f}(t)) \mathcal{L} \left( \exp -\frac{\alpha t}{1-\alpha} \right) = \frac{(\tau \mathcal{L}(f(t)) - f(0))}{\tau + \alpha(1-\tau)}.$$

Similarly,

$$\mathcal{L} [{}^{CF}\mathcal{D}_t^{\alpha+1} f(t)] = \frac{1}{(1-\alpha)} \mathcal{L}(\ddot{f}(t)) \mathcal{L} \left( \exp -\frac{\alpha t}{1-\alpha} \right) = \frac{(\tau^2 \mathcal{L}[f(t)] - \tau f(0) - f'(0))}{\tau + \alpha(1-\tau)}.$$

And finally,

$$\mathcal{L} [{}^{CF}\mathcal{D}_t^{\alpha+n} f(t)] = \frac{1}{(1-\alpha)} \mathcal{L} [f^{n+1}(t)] \mathcal{L} \left( \exp -\frac{\alpha t}{1-\alpha} \right) = \frac{\tau^{n+1} \mathcal{L}[f(t)] - \tau^n f(0) - \tau^{n-1} f'(0) \dots - f^{(n)}(0)}{p + \alpha(1-p)}.$$

### 1.8.3 Fourier Transform of Fractional Gradient, Divergence and Laplacian

For a function  $w(\mathbf{x}) : \mathbb{R}^3 \rightarrow \mathbb{R}$ , the Fourier transform ( $\mathcal{F}$ ) of the fractional gradient is defined as

$$\mathcal{F}(\nabla^\alpha w(\mathbf{x}))(\zeta) = \int_{\mathbb{R}^3} \nabla^\alpha w(\mathbf{x}) \exp[-2\pi i \zeta \cdot \mathbf{x}] d\mathbf{x}.$$

By considering the gradient formula in [20], the Fourier transform is written as

$$\begin{aligned} \mathcal{F}(\nabla^\alpha w)(\zeta) &= \frac{\alpha}{(1-\alpha)\sqrt{\pi^\alpha}} \mathcal{F} \left( \int_{\mathbb{R}^3} \nabla w(\mathbf{y}) \exp \left[ -\frac{\alpha^2(\mathbf{x}-\mathbf{y})^2}{(1-\alpha)^2} \right] d\mathbf{y} \right) (\zeta) \\ &= \frac{\alpha}{(1-\alpha)\sqrt{\pi^\alpha}} \mathcal{F}(\nabla w)(\zeta) \mathcal{F} \left( \exp \left[ -\frac{\alpha^2 \mathbf{x}^2}{(1-\alpha)^2} \right] \right) (\zeta), \end{aligned}$$

where

$$\mathcal{F}\left(\exp\left[-\frac{\alpha^2 \mathbf{x}^2}{(1-\alpha)^2}\right]\right)(\zeta) = \frac{(1-\alpha)\sqrt{\pi}}{\alpha} \exp\left[-\frac{\pi^2(1-\alpha)^2\zeta^2}{\alpha^2}\right].$$

Thus, we get

$$\mathcal{F}(\nabla^\alpha w)(\zeta) = \sqrt{\pi^{1-\alpha}} \mathcal{F}(\nabla w)(\zeta) \exp\left[-\frac{\pi^2(1-\alpha)^2\zeta^2}{\alpha^2}\right].$$

Similarly, the Fourier transform of fractional divergence is given as

$$\begin{aligned} \mathcal{F}(\nabla^\alpha \cdot \mathbf{w})(\zeta) &= \frac{\alpha}{(1-\alpha)\sqrt{\pi^\alpha}} \mathcal{F}\left(\int_{\Omega} \nabla \cdot \mathbf{w}(\mathbf{y}) \exp\left[-\frac{\alpha^2(\mathbf{x}-\mathbf{y})^2}{(1-\alpha)^2}\right] d\mathbf{y}\right)(\zeta) \\ &= \sqrt{\pi^{1-\alpha}} \mathcal{F}(\nabla \cdot \mathbf{w})(\zeta) \exp\left[-\frac{\pi^2(1-\alpha)^2\zeta^2}{\alpha^2}\right]. \end{aligned}$$

By using the definitions of fractional gradient and divergence, one can suggest the representation of the fractional Laplacian for a given function  $f(\mathbf{x}) : \Omega \rightarrow \mathbb{R}^3$ , such that  $\nabla f(\mathbf{x}) \cdot \mathbf{n}|_{\partial\Omega} = 0$ , as

$$(\nabla^2)^\alpha f(\mathbf{x}) = \frac{\alpha}{(1-\alpha)\sqrt{\pi^\alpha}} \int_{\Omega} \nabla \cdot \nabla f(\mathbf{y}) \exp\left[-\frac{\alpha^2(\mathbf{x}-\mathbf{y})^2}{(1-\alpha)^2}\right] d\mathbf{y}.$$

By Theorem 2.1 of [20], we get

$$(\nabla^2)^\alpha f(\mathbf{x}) = \nabla \cdot \nabla^\alpha f(x) = \nabla^\alpha \cdot \nabla f(x).$$

Next, we assume that  $f(x) = 0$ , on  $\partial\Omega$  and consider the Fourier transform

$$\begin{aligned} \mathcal{F}((\nabla^2)^\alpha f(\mathbf{x})) &= \frac{\alpha}{(1-\alpha)\sqrt{\pi^\alpha}} \left(\int_{\mathbb{R}^3} \nabla^2 f(\mathbf{y}) \exp\left[-\frac{\alpha^2(\mathbf{x}-\mathbf{y})^2}{(1-\alpha)^2}\right] d\mathbf{y}\right)(\zeta) \\ &= \frac{\alpha}{(1-\alpha)\sqrt{\pi^\alpha}} \mathcal{F}(\nabla \cdot \nabla f(\mathbf{x}))(\zeta) \mathcal{F}\left(\exp\left[-\frac{\alpha^2 \mathbf{x}^2}{(1-\alpha)^2}\right]\right)(\zeta) \\ &= 4\pi|\zeta|^2 \mathcal{F}(f(\mathbf{x}))(\zeta) \sqrt{\pi^{1-\alpha}} \exp\left[-\frac{(1-\alpha)^2\zeta^2}{\alpha^2}\right] \end{aligned} \quad (1.8.6)$$

substituting for  $\alpha = 1$  in (1.8.6), we have

$$\begin{aligned} \mathcal{F}((\nabla^2) f(\mathbf{x})) &= -\lim_{\alpha \rightarrow 1} 4\pi|\zeta|^2 \mathcal{F}(f(\mathbf{x}))(\zeta) \sqrt{\pi^{1-\alpha}} \exp\left[-\frac{(1-\alpha)^2\zeta^2}{\alpha^2}\right] \\ &= -4\pi|\zeta|^2 \mathcal{F}(f(\mathbf{x}))(\zeta). \end{aligned}$$

### 1.8.4 Caputo–Fabrizio Fractional Derivative in Riemann–Liouville Sense

Let us recall from [35] that the Riemann–Liouville fractional derivative

$${}_a\mathcal{D}_t^\alpha f(t) = \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} \int_a^t f(\tau) \exp\left(-\frac{\alpha}{1-\alpha}(t-\tau)\right) d\tau$$

can be written in the form

$${}_a\mathcal{D}_t^\alpha f(t) = \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} (f(t) * g(t)), \quad (1.8.7)$$

where  $g(t) = \exp\left(-\frac{\alpha t}{1-\alpha}\right)$ , and  $*$  denotes the Laplace convolution operator which defines the convolution integral with the functions

$$f(t) * g(t) = \int_a^t f(\tau)g(t-\tau)d\tau.$$

In what follows and in the spirits of Goufo and Atangana [35], we briefly consider the new Caputo–Fabrizio derivative of the sine function, with application in physics. For instance, we let function  $f(t) = \sin \omega t$ , for general order  $\alpha$  with  $a = 0$  and  $\omega = 1$ , we have

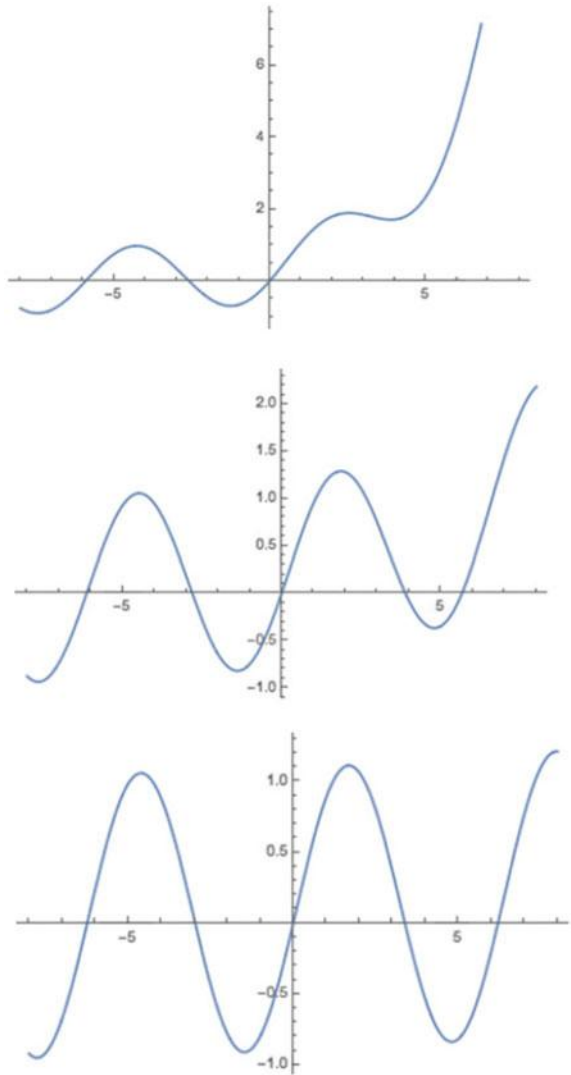
$$\begin{aligned} \mathcal{D}_t^\alpha \sin \omega t &= \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} \int_0^t \sin \tau \exp\left(-\frac{\alpha}{1-\alpha}(t-\tau)\right) d\tau \\ &= \frac{(\alpha-1)\sin t + \alpha \cos t - \alpha \exp\left(\frac{\alpha t}{1-\alpha}\right)}{1+2\alpha(\alpha-1)}. \end{aligned}$$

The results at some instances of  $\alpha$  are displayed in Fig. 1.4. It is obvious that the new derivative exhibits a similar behaviour to the Caputo–Fabrizio fractional derivative [20, 35] for values  $\alpha$  closer to one than  $\alpha$  closer to zero.

Next, we consider the Laplace transform of the Caputo–Fabrizio fractional derivative in Riemann–Liouville sense. Without loss of generality, we let  $a = 0$ , and assume  ${}_0\mathcal{D}_t^\alpha = \mathcal{D}_t^\alpha$ . By using definition (1.8.7) and property of the Laplace transform  $\mathcal{L}(f(t), s)$ , we get

$$\begin{aligned} \mathcal{L}(\mathcal{D}_t^\alpha, s) &= \frac{M(\alpha)}{1-\alpha} \mathcal{L}\left(\frac{d}{dt} \int_0^t f(\tau) \exp\left(-\frac{\alpha}{1-\alpha}(t-\tau)\right) d\tau, s\right) \\ &= \frac{M(\alpha)}{1-\alpha} \mathcal{L}\left(\frac{d}{dt} (f(t) * g(t)), s\right) \\ &= \frac{M(\alpha)}{1-\alpha} [s\mathcal{L}(f(t), s)\mathcal{L}(g(t), s)]. \end{aligned}$$

**Fig. 1.4** Behaviour of function  $\mathcal{D}_t^\alpha \sin \omega t$ ,  $\omega = 1$  at some instances of fractional power  $\alpha$ . Top: when  $\alpha = 0.16$ , middle: when  $\alpha = 0.30$  and bottom panel for  $\alpha = 0.90$



Hence,

$$\mathcal{L}(\mathcal{D}_t^\alpha f(t), s) = \frac{sM(\alpha)}{s + \alpha(1 - s)} \mathcal{L}(f(t), s). \tag{1.8.8}$$

## 1.9 Stretch Fractional Differentiation

Fractional derivative problems with exponential kernels have obvious some limitations when characterizing anomalous relaxation and diffusion of a non-exponential nature [113]. Here, we only report the proposed and legitimate version of the stretched exponential function of Caputo type:

$${}^{Sc}\mathcal{D}^\alpha f(t) = \frac{M(\alpha)}{(1-\alpha)^{1/\alpha}} \int_a^t f'(\tau) \exp\left[-\frac{\alpha(t-\tau)^\alpha}{1-\alpha}\right] d\tau, \quad 0 < \alpha < 1,$$

where  $Sc$  stands for the stretched exponential Caputo definition, and  $M(\alpha)$  is the usual normalization function.

The  $\beta$ -order version of fractional derivative, for  $\beta > 1$  and  $\beta = n + \alpha$ ,  $\alpha \in (0, 1]$  and  $n$  integer is defined as

$${}^{Sc}\mathcal{D}^\beta f(t) = {}^S\mathcal{D}^\alpha f^{(n)}(t) = \frac{M(\alpha)}{(1-\alpha)^{1/\alpha}} \int_a^t f^{(n+1)}(\tau) \exp\left[-\frac{\alpha(t-\tau)^\alpha}{1-\alpha}\right] d\tau.$$

The stretched exponential kernel with strong memory is proposed as

$${}^{Sc}\mathcal{D}^\alpha = \frac{1}{(1-\alpha)^{1/\alpha} \Gamma(1+\alpha)} \int_a^t f'(\tau) \exp\left[-\frac{\alpha}{1-\alpha} \left(\frac{t-\tau}{t}\right)^\alpha\right] d\tau. \quad (1.9.1)$$

Apart from the strong memory, another merit of definition (1.9.1) is that the fractional dimension model in the application of fractional derivative operators can be handled with the introduction of the expression of  $(t-\tau)/t$ , see Sun et al. [113] for details.

## 1.10 The Atangana–Baleanu Fractional Derivative and Integral

In this subsection, we briefly present the definitions and properties of the Atangana–Baleanu fractional derivative and integral in the senses of Caputo and Riemann–Liouville derivatives.

Recall that the Mittag–Leffler function is the solution of equation of the form [9, 46, 52]

$$\frac{d^\alpha u}{dx^\alpha} = au, \quad 0 < \alpha < 1.$$

In the spirit of [9], we consider the generalized Mittag–Leffler function

$$E_\alpha(-t^\alpha) = \sum_{s=0}^{\infty} \frac{(-t)^\alpha s}{\Gamma(\alpha s + 1)}.$$

At point  $t$ , we give the Taylor series of  $\exp[-(t - u)]$  by

$$\exp[-a(t - u)] = \sum_{s=0}^{\infty} \frac{[-a(t - u)]^s}{s!}. \quad (1.10.1)$$

By choosing  $a = a/(1 - \alpha)$  and replacing the expression in the above equation into the Caputo–Fabrizio derivative, we have

$$\mathcal{D}_t^\alpha[f(t)] = \frac{M(\alpha)}{1 - \alpha} \sum_{s=0}^{\infty} \frac{(-a)^s}{s!} \int_a^t \frac{df(u)}{du} [(t - u)]^s du. \quad (1.10.2)$$

The following expression is derived to solve the non-locality problem. In Eq. (1.10.2), we replace  $s!$  by  $\Gamma(\alpha s + 1)$ , similarly let  $(t - u)^s$  be replaced by  $(t - u)^{\alpha s}$  to get

$$\mathcal{D}_t^\alpha[f(t)] = \frac{M(\alpha)}{1 - \alpha} \sum_{s=0}^{\infty} \frac{(-a)^s}{\Gamma(\alpha s + 1)} \int_a^t \frac{df(u)}{du} [(t - u)]^{\alpha s} du.$$

As a result, Atangana and Baleanu [9] proposed the following derivative.

**Definition 1.10.1** Let  $f \in H^1(a, b)$ ,  $a < b$ ,  $\alpha \in [0, 1]$  then, the definition of the Atangana and Baleanu fractional derivative in Caputo sense is given as

$${}^a{}^{ABC}\mathcal{D}_t^\alpha[f(t)] = \frac{M(\alpha)}{1 - \alpha} \int_a^t f'(x) E_\alpha \left[ -\alpha \frac{(t - x)^\alpha}{1 - \alpha} \right] dx, \quad (1.10.3)$$

where  $M(\alpha)$  has the same properties as in the case of the Caputo–Fabrizio fractional derivative.

The above definition is considered to be useful to discuss real-world problems, and it will also be a great advantage when applying the Laplace transform to solve some real-life (physical) models with initial conditions. However, it should be noted that we do not recover the original function when  $\alpha = 0$  except when at the origin the function vanishes. To avoid this kind of problem, the following definition is proposed.

**Definition 1.10.2** Let  $f \in H^1(a, b)$ ,  $a < b$ ,  $\alpha \in [0, 1]$  then, the definition of the Atangana–Baleanu fractional derivative in Riemann–Liouville sense becomes

$${}^a{}^{ABR}\mathcal{D}_t^\alpha[f(t)] = \frac{M(\alpha)}{1 - \alpha} \frac{d}{dt} \int_a^t f(x) E_\alpha \left[ -\alpha \frac{(t - x)^\alpha}{1 - \alpha} \right] dx. \quad (1.10.4)$$

Obviously, both (1.10.3) and (1.10.4) possess a non-local kernel. We also obtain zero whenever the function in Eq. (1.10.3) is constant.

Next, we consider some properties of the Atangana–Baleanu fractional derivatives. We begin by presenting the relation between both derivatives in the senses of

Riemann–Liouville and Caputo with the Laplace transform. By simple calculation, we conclude that

$$\mathcal{L}\{ {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)]\}(q) = \frac{M(\alpha)}{1-\alpha} \frac{q^\alpha \mathcal{L}\{f(t)\}(q)}{q^\alpha + \frac{\alpha}{1-\alpha}} \quad (1.10.5)$$

and

$$\mathcal{L}\{ {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)]\}(q) = \frac{M(\alpha)}{1-\alpha} \frac{q^\alpha \mathcal{L}\{f(t)\}(q) - q^{\alpha-1} f(0)}{q^\alpha + \frac{\alpha}{1-\alpha}} \quad (1.10.6)$$

are the Laplace transform for the respective derivatives. Hence, we establish the following theorem.

**Theorem 1.10.3** *Let  $f \in H^1(a, b)$ ,  $a < b$ ,  $\alpha \in [0, 1]$  then, the following relation is obtained*

$${}_0^{ABC}\mathcal{D}_t^\alpha[f(t)] = {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)] + H(t). \quad (1.10.7)$$

*Proof* By applying the Laplace transform to both sides of the relation (1.10.7), we easily obtain the result

$$\mathcal{L}\{ {}_0^{ABC}\mathcal{D}_t^\alpha[f(t)]\}(q) = \frac{M(\alpha)}{1-\alpha} \frac{q^\alpha \mathcal{L}\{f(t)\}(q)}{q^\alpha + \frac{\alpha}{1-\alpha}} - \frac{q^{\alpha-1} f(0)}{q^\alpha + \frac{\alpha}{1-\alpha}} \frac{M(\alpha)}{1-\alpha}.$$

From (1.10.5), we obtain

$$\mathcal{L}\{ {}_0^{ABC}\mathcal{D}_t^\alpha[f(t)]\}(q) = \mathcal{L}\{ {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)]\}(q) - \frac{q^{\alpha-1} f(0)}{q^\alpha + \frac{\alpha}{1-\alpha}} \frac{M(\alpha)}{1-\alpha}. \quad (1.10.8)$$

By applying the inverse Laplace transform on both sides of (1.10.8), we have

$${}_0^{ABC}\mathcal{D}_t^\alpha[f(t)] = {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)] - \frac{M(\alpha)}{1-\alpha} f(0) E_\alpha\left(-\frac{\alpha}{1-\alpha} t^\alpha\right).$$

The proof is completed.  $\square$

**Theorem 1.10.4** *Let  $f$  be a continuous function on  $[a, b]$ . Then, the following inequality is satisfied on a closed interval  $[a, b]$ :*

$$\| {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)] \| < \frac{M(\alpha)}{1-\alpha} B, \quad \|g(t)\| = \max_{a \leq t \leq b} |g(t)|.$$

*Proof*

$$\begin{aligned}\| {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)] \| &= \left\| \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} \int_0^t f(x) E_\alpha \left[ -\alpha \frac{(t-x)^\alpha}{1-\alpha} \right] dx \right\| < \frac{M(\alpha)}{1-\alpha} \left\| \frac{d}{dt} \int_0^t f(x) dx \right\|, \\ &= \frac{M(\alpha)}{1-\alpha} \|f(x)\|.\end{aligned}$$

The proof is completed whenever  $B$  is taking to  $\|f(x)\|$ .  $\square$

**Theorem 1.10.5** *The Atangana–Baleanu fractional derivative in senses Riemann–Liouville and Caputo satisfy the Lipschitz condition, for the given functions  $f$  and  $g$ , the following inequalities can be obtained:*

$$\| {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)] - {}_0^{ABR}\mathcal{D}_t^\alpha[g(t)] \| \leq H \|f(t) - g(t)\| \quad (1.10.9)$$

and

$$\| {}_0^{ABC}\mathcal{D}_t^\alpha[f(t)] - {}_0^{ABC}\mathcal{D}_t^\alpha[g(t)] \| \leq H \|f(t) - g(t)\|. \quad (1.10.10)$$

Here the proof of (1.10.9) is given as that of (1.10.10). It can also be obtained vice versa.

*Proof*

$$\begin{aligned}\| {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)] - {}_0^{ABR}\mathcal{D}_t^\alpha[g(t)] \| &= \left\| \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} \int_0^t f(x) E_\alpha \left[ -\alpha \frac{(t-x)^\alpha}{1-\alpha} \right] dx \right. \\ &\quad \left. - \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} \int_0^t g(x) E_\alpha \left[ -\alpha \frac{(t-x)^\alpha}{1-\alpha} \right] dx \right\|.\end{aligned}$$

By using the Lipschitz condition of the first derivative, it is possible to find a small constant, such that

$$\| {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)] - {}_0^{ABR}\mathcal{D}_t^\alpha[g(t)] \| < \frac{M(\alpha)\phi_1}{1-\alpha} E_\alpha \left( -\alpha \frac{t^\alpha}{1-\alpha} \right) \left\| \int_0^t f(x) dx - \int_0^t g(x) dx \right\|$$

and we obtain the following results

$$\begin{aligned}\| {}_0^{ABR}\mathcal{D}_t^\alpha[f(t)] - {}_0^{ABR}\mathcal{D}_t^\alpha[g(t)] \| &< \frac{M(\alpha)\phi_1}{1-\alpha} E_\alpha \left( -\alpha \frac{t^\alpha}{1-\alpha} \right) \|f(x) - g(x)\| t \\ &= H \|f(x) - g(x)\|\end{aligned}$$

which leads to the required result.  $\square$

Let  $f$  be  $n$ -times differentiable function with natural number  $f^{(s)}(0) = 0$ ,  $s = 1, 2, \dots, n$ , then by inspection we have

$${}_0^{ABC}\mathcal{D}_t^\alpha \frac{d^n f(x)}{dt^n} = \frac{d^n}{dt^n} \{ {}_0^{ABC}\mathcal{D}_t^\alpha [f(t)] \}.$$

Taking the inverse Laplace transform and using the convolution theorem, we can prove that the time-fractional ordinary differential equation

$${}^ABC\mathcal{D}_t^\alpha[f(t)] = \omega(t)$$

possesses a unique solution of the form

$$f(t) = \frac{1-\alpha}{M(\alpha)}\omega(t) + \frac{\alpha}{M(\alpha)\Gamma(\alpha)} \int_0^t \omega(u)(t-u)^{\alpha-1} du.$$

**Definition 1.10.6** The Atangana–Baleanu fractional integral of order  $\alpha$  with base point  $a$  with non-local kernel is defined as

$${}^{AB}\mathcal{I}_t^\alpha\{f(t)\} = \frac{1-\alpha}{M(\alpha)}f(t) + \frac{\alpha}{M(\alpha)\Gamma(\alpha)} \int_a^t f(u)(t-u)^{\alpha-1} du.$$

When  $\alpha = 0$ , we obtain the initial function, and for  $\alpha = 1$ , we get the ordinary integral.

## 1.11 The Riesz Potential and Riesz Fractional Derivatives

Let  $0 < \alpha < 1$ . We consider the following integrals:

$$\mathcal{R}^\alpha f(x) = \frac{1}{2\Gamma(\alpha)\cos\frac{\alpha\pi}{2}} \int_{-\infty}^{\infty} \frac{1}{|x-\tau|^{1-\alpha}} f(\tau) d\tau, \quad x \in \mathbb{R}, \quad (1.11.1)$$

$$\mathcal{H}^\alpha f(x) = \frac{1}{2\Gamma(\alpha)\sin\frac{\alpha\pi}{2}} \int_{-\infty}^{\infty} \frac{\text{sgn}(x-\tau)}{|x-\tau|^{1-\alpha}} f(\tau) d\tau, \quad x \in \mathbb{R}, \quad (1.11.2)$$

where  $\mathcal{R}^\alpha f$  and  $\mathcal{H}^\alpha f$  are known to be the respective Riesz potential and the conjugate Riesz potential of the order  $\alpha$  on  $\mathbb{R}$  [6, 52, 98]. The following proposition is satisfied for Eq. (1.11.2).

**Proposition 1.11.1** ([6, 118]) *The Riemann–Liouville fractional integral and the Riesz potential, for  $x \in \mathbb{R}$ , are connected by the following relations:*

$$\begin{aligned} -\infty\mathcal{I}_x^\alpha f(x) &= \cos\frac{\alpha\pi}{2}\mathcal{R}^\alpha f(x) + \sin\frac{\alpha\pi}{2}\mathcal{H}^\alpha f(x), \\ \infty\mathcal{I}_x^\alpha f(x) &= \cos\frac{\alpha\pi}{2}\mathcal{R}^\alpha f(x) - \sin\frac{\alpha\pi}{2}\mathcal{H}^\alpha f(x), \\ \mathcal{R}^\alpha f(x) &= \frac{1}{2\cos\frac{\alpha\pi}{2}} \left( -\infty\mathcal{I}_x^\alpha f(x) + \infty\mathcal{I}_x^\alpha f(x) \right), \\ \mathcal{H}^\alpha f(x) &= \frac{1}{2\sin\frac{\alpha\pi}{2}} \left( -\infty\mathcal{I}_x^\alpha f(x) - \infty\mathcal{I}_x^\alpha f(x) \right). \end{aligned}$$

Again, if  $\alpha > 0$ ,  $\beta > 0$  and  $\alpha + \beta < 1$ , then

$$\mathcal{R}^\alpha \mathcal{R}^\beta f(x) = \mathcal{R}^{\alpha+\beta} f(x) \quad \text{and} \quad \mathcal{H}^\alpha \mathcal{H}^\beta f(x) = -\mathcal{H}^{\alpha+\beta} f(x), \quad x \in \mathbb{R}.$$

With appropriate assumptions on  $f$ , the integrals (1.11.1) and (1.11.2).

**Proposition 1.11.2** ([52]) *Let  $1 \leq r \leq \infty$  and  $1 \leq s \leq \infty$ . Then,  $\mathcal{R}^\alpha$  is a bounded operator from  $L^r(\mathbb{R})$  into  $L^s(\mathbb{R})$  provided*

$$0 < \alpha < 1, \quad 1 < r < \frac{1}{\alpha}, \quad \frac{1}{s} = \frac{1}{r} - \frac{1}{\alpha}.$$

The Fourier transforms of  $\mathcal{R}^\alpha$  and  $\mathcal{H}^\alpha$  are, respectively, given as

$$\mathcal{F}[\mathcal{R}^\alpha f(x)](\varphi) = \frac{1}{|\varphi|^\alpha} \hat{f}(\varphi)$$

and

$$\mathcal{F}[\mathcal{H}^\alpha f(x)](\varphi) = \frac{-i \operatorname{sgn}(\varphi)}{|\varphi|^\alpha} \hat{f}(\varphi), \quad \varphi \in \mathbb{R},$$

see Butzer and Westphal [17] for details.

**Definition 1.11.3** ([17, 98, 118]) The Riesz fractional derivative of order  $\alpha$  is defined as

$${}^R\mathcal{D}^\alpha f(x) = \frac{d}{dx} \mathcal{H}^{1-\alpha} f(x) = \frac{1}{2\Gamma(1-\alpha) \cos \frac{\alpha\pi}{2}} \frac{d}{dx} \int_{-\infty}^{\infty} \frac{\operatorname{sgn}(x-\tau)}{|x-\tau|^\alpha} f(\tau) d\tau, \quad x \in \mathbb{R}, \quad (1.11.3)$$

and the conjugate Riesz derivative of order  $\alpha$  is given by

$${}^{Rc}\mathcal{D}^\alpha f(x) = \frac{d}{dx} \mathcal{R}^{1-\alpha} f(x) = \frac{1}{2\Gamma(1-\alpha) \sin \frac{\alpha\pi}{2}} \frac{d}{dx} \int_{-\infty}^{\infty} \frac{1}{|x-\tau|^\alpha} f(\tau) d\tau, \quad x \in \mathbb{R}. \quad (1.11.4)$$

The Fourier transforms of (1.11.3) and (1.11.4) for  $\alpha \in (0, 1)$  are presented as

$$\mathcal{F}[{}^R\mathcal{D}^\alpha f(x)](\varphi) = |\varphi|^\alpha \hat{f}(\varphi)$$

and

$$\mathcal{F}[{}^{Rc}\mathcal{D}^\alpha f(x)](\varphi) = i|\varphi|^\alpha \operatorname{sgn}(\varphi) \hat{f}(\varphi), \quad \varphi \in \mathbb{R}$$

respectively, which means that  ${}^R\mathcal{D}^\alpha$  inverts  $\mathcal{R}^\alpha$ , and  ${}^{Rc}\mathcal{D}^\alpha$  inverts  $\mathcal{H}^\alpha$ , provided the involved functions satisfied some additional conditions [17, 110].

### 1.11.1 The Atangana–Gómez Fractional Derivative

The branch of applied mathematics (such as physics, statistics, economics and finance) finds its application in scientific, social and industrial problems. One of the most used tools in applied statistical tool is perhaps the concept of distributions. The normal distribution is an important tool in statistics and also found useful in no small measure in areas of applied natural science and social sciences to portray the distribution of unknown real-valued random variables. The existence of the normal distribution in practical problem has been reported in many fields, for example, in biology, the well-known logarithm of many variables converge to the shape of normal distribution, which is, they converge to log-normal distribution observed after separation on male and female subpopulations which is in other way include measures of size of living tissue in particular their height, length, weight and skin area, see [10] for further illustration.

Another physical problem in biology is the length of inert supplements, for example, claws, hair, nails and teeth of given biotic specimens, of course in the direction of growth; presumably the thickness of tree back also falls under category [81]. Additionally talking of certain physiological measurements like blood pressure of adult humans. In mathematical finance, specifically speaking the Black–Scholes model changes in Logarithm of exchange rates, where both the price and stock market indices are assumed to follow the normal distribution [25]. A keen observation of a natural problem following the normal law is the distribution of long duration liberation or rainfall monthly or yearly totals. Many other physical occurrences can be mentioned. In what follows, we shall present the definitions and properties of the new derivative proposed by Atangana and Gómez [10].

**Definition 1.11.4** Let  $u$  be an  $n$ -differentiable function on interval  $(a, b)$ , then the derivative of  $u$  with averaging kernel of order  $n - 1 < \alpha \leq n$  is defined by

$${}^{AGAC}D_t^\alpha\{u(t)\} = \frac{AG(\alpha)}{n - \alpha} \int_a^t u^n(\tau) \exp\left[-\frac{\alpha}{n - \alpha}(t - \tau)^2\right] d\tau, \quad (1.11.5)$$

where  $\frac{d^\alpha}{dt^\alpha} = {}^{AGAC}D_t^\alpha$  denotes the Atangana–Gómez Averaging fractional derivative in Liouville–Caputo sense with respect to  $t$  and the term  $AG(\alpha)$  is a normalization function.

**Definition 1.11.5** Let  $u$  be a non-differentiable continuous function on interval  $(a, b)$ , then the derivative of  $u$  with averaging kernel of order  $n - 1 < \alpha \leq n$  is defined by

$${}^{AGAR}D_t^\alpha\{u(t)\} = \frac{AG(\alpha)}{n - \alpha} \frac{d^n}{dt^n} \int_a^t u(\tau) \exp\left[-\frac{\alpha}{n - \alpha}(t - \tau)^2\right] d\tau, \quad (1.11.6)$$

where  $\frac{d^\alpha}{dt^\alpha} = {}_a^{AGAR} \mathcal{D}_t^\alpha$  denotes the Atangana–Gómez Averaging fractional derivative in Riemann–Liouville sense with respect to  $t$  and the function  $AG(\alpha)$  is a normalized type.

**Theorem 1.11.6** *The Laplace transform of (1.11.5) yields*

$$\mathcal{L} \left\{ {}_0^{AGAC} \mathcal{D}_t^\alpha \{u(t)\} \right\} = \frac{AG(\alpha)}{1-\alpha} [sU(s) - u(0)] \cdot \left( \frac{1}{s} \right)_2 \Phi_1 \left[ \begin{matrix} (1, 2), (1, 1) \\ (1, 1); \end{matrix} \quad -\frac{\alpha}{1-\alpha} \cdot \frac{1}{s^2} \right], \quad (1.11.7)$$

where the function  ${}_a \Phi_b$  denotes the Wright's generalized hyper-geometric function [73].

*Proof* See Atangana and Gómez [10]. □

**Theorem 1.11.7** *The Laplace transform of (1.11.6) yields*

$$\begin{aligned} \mathcal{L} \left\{ {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} \right\} &= \frac{AG(\alpha)}{1-\alpha} U(s) \cdot {}_2 \Phi_1 \\ &\times \left[ \begin{matrix} (1, 2), (1, 1) \\ (1, 1); \end{matrix} \quad -\frac{\alpha}{1-\alpha} \cdot \frac{1}{s^2} \right]. \end{aligned}$$

**Theorem 1.11.8** *The Sumudu transform of (1.11.5) gives*

$$\begin{aligned} ST \left\{ {}_0^{AGAC} \mathcal{D}_t^\alpha \{u(t)\} \right\} &= \frac{AG(\alpha)}{1-\alpha} [ST\{U(t) - u(0)\}] \cdot {}_2 \Phi_1 \\ &\times \left[ \begin{matrix} (1, 2), (1, 1) \\ (1, 1); \end{matrix} \quad -\frac{\alpha}{1-\alpha} \cdot v^2 \right]. \end{aligned}$$

**Theorem 1.11.9** *The Sumudu transform of (1.11.6) gives*

$$ST \left\{ {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} \right\} = \frac{AG(\alpha)}{1-\alpha} \frac{ST\{U(t)\}}{v} \cdot {}_2 \Phi_1 \left[ \begin{matrix} (1, 2), (1, 1) \\ (1, 1); \end{matrix} \quad -\frac{\alpha}{1-\alpha} \cdot v^2 \right]. \quad (1.11.8)$$

**Theorem 1.11.10** *The Fourier transform of (1.11.5) gives*

$$\mathcal{F} \left\{ {}_0^{AGAC} \mathcal{D}_t^\alpha \{u(t)\} \right\} = \frac{AG(\alpha)}{1-\alpha} (ik) \mathcal{F}\{u(t)\} \sqrt{\frac{\pi}{a}} \left[ \exp \left( -\frac{k^2}{4a} \right) \right], \quad (1.11.9)$$

where  $a = \frac{1-\alpha}{\alpha}$ .

**Theorem 1.11.11** *The Fourier transform of (1.11.6) gives*

$$\mathcal{F} \left\{ {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} \right\} = \frac{AG(\alpha)}{1-\alpha} U(k) \sqrt{\frac{\pi}{a}} \left[ \exp \left( -\frac{k^2}{4a} \right) \right], \quad (1.11.10)$$

where  $a = \frac{1-\alpha}{\alpha}$ .

**Theorem 1.11.12** *The Mellin transform of (1.11.5) gives*

$$\mathfrak{M} \left\{ {}_0^{AGAC} \mathcal{D}_t^\alpha \{u(t)\} \right\} = \frac{AG(\alpha)}{1-\alpha} (s-1) \mathfrak{M}(s-1) \times \frac{\Gamma(s/2)}{2a^{s/2}}, \quad (1.11.11)$$

where  $a = \frac{1-\alpha}{\alpha}$ .

**Theorem 1.11.13** *The Mellin transform of (1.11.6) gives*

$$\mathfrak{M} \left\{ {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} \right\} = \frac{AG(\alpha)}{1-\alpha} \mathfrak{M}(s) \times \frac{\Gamma(s/2)}{2a^{s/2}}, \quad (1.11.12)$$

where  $a = \frac{1-\alpha}{\alpha}$ .

**Theorem 1.11.14** *Let  $u$  be a continuous function, such that  ${}_0^{AGAR} \mathcal{D}_t^\alpha \{f(t)\}$  exists then, for  $0 < \alpha \leq 1$ , the following equation*

$${}_0^{AGAR} \mathcal{D}_t^\alpha \{f(t)\} = v(t)$$

*has unique solution.*

*Proof* By applying the Fourier transform on both sides of above equation, we obtain

$$\begin{aligned} (\mathcal{F})[v(t)] &= \frac{AG(\alpha)}{1-\alpha} i\chi(\mathcal{F})[u(t)] \cdot (\mathcal{F}) \left[ \exp \left( -\frac{\alpha}{1-\alpha} t^2 \right) \right], \\ (\mathcal{F})[v(t)] &= \frac{AG(\alpha)}{1-\alpha} i\chi(\mathcal{F})[u(t)] \left[ \frac{1}{\sqrt{2}\sqrt{\frac{\alpha}{1-\alpha}}} \right] \left[ \exp \left( \chi^2 \frac{\alpha-1}{4\alpha} t^2 \right) \right], \\ (\mathcal{F})[v(t)] &= \sqrt{2}\sqrt{\frac{\alpha}{1-\alpha}} (\mathcal{F})[v(t)] \left( \frac{1}{i\chi} \right) \left( \frac{1-\alpha}{AG(\alpha)} \right) \left[ \frac{\chi^2(1-\alpha)}{4\alpha} \right]. \end{aligned}$$

Using the inverse Fourier transform in conjunction with convolution theorem, we have

$$\begin{aligned}
 u(t) &= -\sqrt{2}\sqrt{\frac{\alpha}{1-\alpha}} \int_0^t v(\tau) \left( \frac{1-\alpha}{AG(\alpha)} \right) \cdot \left( \sqrt{\frac{\pi}{2}} \right) \operatorname{erfc} \left[ \frac{t-\tau}{2\sqrt{\frac{\alpha-1}{\alpha}}} \right] d\tau, \\
 &= \frac{\sqrt{2\alpha(1-\alpha)}}{\sqrt{AG(\alpha)}} \int_0^t v(\tau) \operatorname{erfc} \left[ -\frac{t-\tau}{2\sqrt{\frac{\alpha-1}{\alpha}}} \right] d\tau,
 \end{aligned}$$

the  $\operatorname{erfc}(\cdot)$  represents the error function given in [43].  $\square$

**Definition 1.11.15** Let  $u$  be a continuous function defined on  $(a, b)$ , then the Atangana–Gómez Averaging integral of  $u$  with order  $\alpha$  is defined by

$${}_0^{AGAR} \mathbf{I}_t^\alpha \{u(t)\} = \frac{\sqrt{2\alpha(1-\alpha)}}{\sqrt{AG(\alpha)}} \int_0^t v(\tau) \operatorname{erfc} \left[ -\frac{t-\tau}{2\sqrt{\frac{\alpha-1}{\alpha}}} \right] d\tau. \quad (1.11.13)$$

**Theorem 1.11.16** Let  $u$  and  $v$  be two continuous functions for which  ${}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\}$  and  ${}_0^{AGAR} \mathcal{D}_t^\alpha \{v(t)\}$  exist. There exists a positive real number  $c$  such that

$$\left\| {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} - {}_0^{AGAR} \mathcal{D}_t^\alpha \{v(t)\} \right\| \leq c \|u(t) - v(t)\|.$$

*Proof*

$$\begin{aligned}
 &\left\| {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} - {}_0^{AGAR} \mathcal{D}_t^\alpha \{v(t)\} \right\| \\
 &= \frac{AG(\alpha)}{1-\alpha} \left\| \frac{d}{dt} \int_0^t \left\{ u(\tau) \exp \left[ -\frac{\alpha}{1-\alpha} (t-\tau)^2 \right] - v(\tau) \exp \left[ -\frac{\alpha}{1-\alpha} (t-\tau)^2 \right] \right\} d\tau \right\| \\
 &\leq \frac{AG(\alpha)}{1-\alpha} \varpi_1 \int_0^t \|u(t) - v(t)\| \exp \left[ -\frac{\alpha}{1-\alpha} (t-\tau)^2 \right] d\tau, \\
 &\leq \frac{AG(\alpha)}{1-\alpha} \varpi_1 \left( \frac{1}{2} \sqrt{\pi} \right) \left( \sqrt{\frac{\alpha-1}{\alpha}} \right) \operatorname{erfc} \left[ i \left( -\frac{t}{\sqrt{\frac{\alpha-1}{\alpha}}} \right) \right] \|u(t) - v(t)\|, \\
 &\leq \mathfrak{K} \|u(t) - v(t)\|,
 \end{aligned}$$

where

$$\mathfrak{K} = \frac{AG(\alpha)}{1-\alpha} \varpi_1 \left( \frac{1}{2} \sqrt{\pi} \right) \left( \sqrt{\frac{\alpha-1}{\alpha}} \right) \operatorname{erfc} \left[ i \left( -\frac{t}{\sqrt{\frac{\alpha-1}{\alpha}}} \right) \right].$$

The proof is completed.  $\square$

**Theorem 1.11.17** Let  $u$  be a continuous function such that  ${}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\}$  exists, then

$${}_0^{AGAC} \mathcal{D}_t^\alpha \{u(t)\} = {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} + g(t).$$

*Proof*

$$\begin{aligned}
 & \mathcal{L} \left\{ {}_0^{AGAC} \mathcal{D}_t^\alpha \{u(t)\} \right\} \\
 &= \frac{AG(\alpha)}{1-\alpha} \mathcal{L} \left\{ \exp \left[ -\frac{\alpha}{1-\alpha} t^2 \right] \right\} \\
 &= \frac{AG(\alpha)}{1-\alpha} \frac{(\nabla \mathcal{L}\{u(t)\} - u(0))}{2\sqrt{\frac{\alpha}{\pi-\alpha\pi}}} \cdot \exp \left[ -\nabla^2 \left( \frac{\alpha-1}{4\alpha} \right) \right] \operatorname{erfc} \left[ \frac{\nabla}{2\sqrt{\frac{\alpha}{\pi-\alpha\pi}}} \right], \\
 &= \frac{AG(\alpha)}{1-\alpha} \frac{\mathcal{L}\{u(t)\}}{2\sqrt{\frac{\alpha}{\pi-\alpha\pi}}} \exp \left[ -\nabla^2 \left( \frac{\alpha-1}{4\alpha} \right) \right] \operatorname{erfc} \left[ \frac{\nabla}{2\sqrt{\frac{\alpha}{\pi-\alpha\pi}}} \right] \\
 &\quad - \frac{AG(\alpha)}{1-\alpha} \frac{u(0)}{2\sqrt{\frac{\alpha}{\pi-\alpha\pi}}} \exp \left[ -\nabla^2 \left( \frac{\alpha-1}{4\alpha} \right) \right] \operatorname{erfc} \left[ \frac{\nabla}{2\sqrt{\frac{\alpha}{\pi-\alpha\pi}}} \right] \\
 &= \mathcal{L} \left\{ {}_0^{AGAC} \mathcal{D}_t^\alpha \{u(t)\} \right\} - \\
 &\quad \frac{AG(\alpha)}{1-\alpha} \frac{u(0)}{2\sqrt{\frac{\alpha}{\pi-\alpha\pi}}} \exp \left[ -\nabla^2 \left( \frac{\alpha-1}{4\alpha} \right) \right] \operatorname{erfc} \left[ \frac{\nabla}{2\sqrt{\frac{\alpha}{\pi-\alpha\pi}}} \right].
 \end{aligned}$$

By taking the inverse Laplace transform produces

$$\begin{aligned}
 {}_0^{AGAC} \mathcal{D}_t^\alpha \{u(t)\} &= {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} - \frac{AG(\alpha)}{1-\alpha} f(0) \exp \left[ -\frac{\alpha}{1-\alpha} t^2 \right], \\
 &= {}_0^{AGAR} \mathcal{D}_t^\alpha \{u(t)\} + g(t).
 \end{aligned}$$

The proof is completed.  $\square$

**Theorem 1.11.18** *Let  $u$  be a continuous and bounded function in an interval  $(a, b)$ , then the Atangana–Gómez averaging integral satisfies*

$$\left\| {}_0^{AGA} \mathbf{I}_t^\alpha \{u(t)\} \right\| \leq \frac{AG(\alpha)}{1-\alpha} M \mathfrak{K}_1.$$

*Proof*

$$\left\| {}_0^{AGA} \mathbf{I}_t^\alpha \{u(t)\} \right\| \leq \frac{\sqrt{2\alpha(1-\alpha)}}{AG(\alpha)} \int_0^t \|u(\tau)\| \left\| \operatorname{erfc} \left[ -\frac{t-\tau}{2\sqrt{\frac{\alpha-1}{\alpha}}} \right] \right\| d\tau.$$

Since  $u$  is bounded, we can set  $M < \infty$  such that  $\|u(t)\| \leq M$ , where  $t \in (a, b)$ , then

$${}_0^{AGA}\mathbf{I}_t^\alpha\{u(t)\} \leq \frac{\sqrt{2\alpha(1-\alpha)}}{AG(\alpha)} \mathbb{M} \int_0^t \operatorname{erfc} \left[ -\frac{t-\tau}{2\sqrt{\frac{\alpha-1}{\alpha}}} \right] d\tau,$$

where

$$\int_0^t \operatorname{erfc} \left[ -\frac{t-\tau}{2\sqrt{\frac{\alpha-1}{\alpha}}} \right] d\tau = \frac{2 \left( -\exp \left[ \frac{\alpha}{4-4\alpha} t^2 \right] + 1 \right) \sqrt{\frac{\alpha-1}{\alpha}} + (\sqrt{\pi t}) \operatorname{erfc} \left[ -\frac{t-\tau}{2\sqrt{\frac{\alpha-1}{\alpha}}} \right]}{\sqrt{\pi}},$$

hence, we can obtain  $\mathfrak{K}_1$  such that  $t \in (a, b)$

$$2 \left( -\exp \left[ \frac{\alpha}{4-4\alpha} t^2 \right] + 1 \right) \sqrt{\frac{\alpha-1}{\alpha}} + (\sqrt{\pi t}) \operatorname{erfc} \left[ -\frac{t-\tau}{2\sqrt{\frac{\alpha-1}{\alpha}}} \right] < \mathfrak{K}_1.$$

Then

$$\|{}_0^{AGA}\mathbf{I}_t^\alpha\{u(t)\}\| \leq \frac{AG(\alpha)}{1-\alpha} \mathbb{M} \mathfrak{K}_1.$$

This completes the proof.  $\square$

## References

1. N.H. Abel, Auflösung einer mechanischen Aufgabe. *Journal für reine und angewandte Mathematik* **1**, 153–157 (1826)
2. N.H. Abel, Solution de quelques problèmes à l'aide d'intégrales définies. *Oeuvres Complètes* **1**, 16–18 (1881)
3. R.P. Agarwal, A propos d'une note de M. Pierre Humbert, *C. R. Séances Acad. Sci.*, **236**, 2031–2032 (1953)
4. O.P. Agrawal, Generalized variational problems and Euler-Lagrange equations. *Comput. Math. Appl.* **59**, 1852–1864 (2010)
5. A. Almeida, S. Samko, Fractional and hypersingular operators in variable exponent spaces on metric measure spaces. *Mediterranean J. Math.* **6**, 215–232 (2009)
6. T.M. Atanacković, S. Pilipović, B. Stanković, D. Zorica, *Fractional Calculus with Applications in Mechanics* (John Wiley & Sons Inc, Hoboken, USA, 2014)
7. A. Atangana, A. Secer, A note on fractional order derivatives and table of fractional derivatives of some special functions. *Abstract Appl. Anal.* **2013**, 8 p. (2013). <https://doi.org/10.1155/2013/279681>
8. A. Atangana, On the new fractional derivative and application to nonlinear Fisher's reaction-diffusion equation. *Appl. Math. Comput.* **273**, 948–956 (2016)
9. A. Atangana, D. Baleanu, New fractional derivatives with non-local and non-singular kernel: theory and application to heat transfer model. *Thermal Sci.* **20**, 763–769 (2016)
10. A. Atangana, J.F. Gómez-Aguilar, A new derivative with normal distribution kernel: theory, methods and applications. *Physica A* **476**, 1–14 (2017)

11. A. Atangana, I. Koca, Chaos in a simple nonlinear system with Atangana-Baleanu derivatives with fractional order. *Chaos Solitons Fractals* **89**, 447–454 (2016)
12. B. Baeumer, M.M. Meerschaert, Tempered stable Lévy motion and transient super-diffusion. *J. Comput. Appl. Math.* **233**, 243–248 (2010)
13. T. Bakkyaraj, R. Sahadevan, Invariant analysis of nonlinear fractional ordinary differential equations with Riemann-Liouville fractional derivative. *Nonlinear Dyn.* **80**, 447–455 (2015)
14. L. Bourdin, T. Odziejewicz, D.F.M. Torres, Existence of minimizers for generalized Lagrangian functionals and a necessary optimality condition-application to fractional variational problems. *Differ. Integral Equ.* **27**, 743–766 (2014)
15. D. Brockmann, L. Hufnagel, T. Geisel, The scaling laws of human travel. *Nature* **439**(2006), 462–465 (2006)
16. A. Bueno-Orovio, D. Kay, K. Burrage, Fourier spectral methods for fractional-in-space reaction-diffusion equations. *BIT Numer. Math.* **54**, 937–954 (2014)
17. P.I. Butzer, U. Westphal, An introduction to fractional calculus, in *Applications of Fractional Calculus in Physics*, ed. by R. Hilfer (World Scientific, Singapore, 2000), pp. 1–85
18. M. Caputo, Linear models of dissipation whose  $Q$  is almost frequency independent II. *Geophys. J. Royal Astron. Soc.* **13**, 529–539 (1967)
19. M. Caputo, *Elasticita e Dissipazione* (Zanichelli, Bologna, 1969)
20. M. Caputo, M. Fabrizio, A new definition of fractional derivative without singular kernel. *Progress Fract. Diff. Appl.* **1**, 73–85 (2015)
21. M. Caputo, M. Fabrizio, Applications of new time and spatial fractional derivatives with exponential kernels. *Progress Fract. Differ. Appl.* **2**, 1–11 (2016)
22. A. Cartea, D. del-Castillo-Negrete, Fractional diffusion models of option prices in markets with jumps. *Phys. A*, **374**, 749–763 (2007)
23. J. Chen, Z. Zeng, P. Jiang, Global Mittag-Leffler stability and synchronization of memristor-based fractional-order neural networks. *Neural Netw.* **51**, 1–8 (2014)
24. C.F.M. Coimbra, Mechanics with variable-order differential operators. *Ann. Phys.* **12**, 692–703 (2003)
25. C. Conrick, S. Hanson, Normal distribution. *Probab. Modern Financ. Theory* **1**, 93–109 (2013)
26. J. Cresson, Fractional embedding of differential operators and Lagrangian systems. *J. Math. Phys.* **48** 033504, 34 p. (2007)
27. E.C. de Oliveira and J.A.T. Machado, A Review of Definitions for fractional derivatives and integral. *Math. Problems Eng.* **2014** (2014) Article ID 238459, 6 p., <https://doi.org/10.1155/2014/238459>
28. J. Deng, L. Zhao, Y. Wu, Fast predictor-corrector approach for the tempered fractional ordinary differential equations. *Numer. Algorithms* **74**, 717–754 (2017)
29. G. Diaz, C.F.M. Coimbra, Nonlinear dynamics and control of a variable order oscillator with application to the van der Pol equation. *Nonlinear Dyn.* **56**, 145–157 (2009)
30. K. Diethelm, *The Analysis of Fractional Differential Equations: An Application-oriented Exposition using Differential Operators of Caputo type* (Springer Lecture Notes in Mathematics, Springer, Berlin Heidelberg, 2010)
31. A. Erdélyi, On fractional integration and its application on the theory of Hankel transforms. *Quart. J. Math.* **11**, 293–303 (1940)
32. A. Erdélyi, H. Kober, Some remarks on Hankel transforms. *Quart. J. Math.* **11**, 212–221 (1940)
33. B.A. Faycal, About Non-differentiable functions. *J. Math. Anal. Appl.* **263**, 721–737 (2001)
34. R. Friedrich, F. Jenko, A. Baule, S. Eule, Anomalous diffusion of inertial, weakly damped particles. *Phys. Rev. Lett.* **96**, 230601 (2006)
35. E.F.D. Goufo, A. Atangana, Analytical and numerical schemes for a derivative with filtering property and no singular kernel with applications to diffusion. *Eur. Phys. J. Plus* **131**, 269 (2016). <https://doi.org/10.1140/epjp/i2016-16269-1>
36. I. Goychuk, V.O. Kharchenko, R. Metzler, Molecular motors pulling cargos in the viscoelastic cytosol: how power strokes beat subdiffusion. *Phys. Chem. Chem. Phys.* **16**, 16524–16535 (2014)

37. I. Gradshteyn, I. Ryzhik, *Table of Integrals, Series, and Products* (Academic Press, New York, 1980)
38. D.S. Grebenkov, M. Vahabi, E. Bertseva, L. Forró, S. Jeney, Hydrodynamic and subdiffusive motion of tracers in a viscoelastic medium. *Phys. Rev. E* **88**, 071 (2013)
39. D.S. Grebenkov, M. Vahabi, E. Bertseva, L. Forró, S. Jeney, Hydrodynamic and subdiffusive motion of tracers in a viscoelastic medium. *Phys. Rev. E* **88**, 071 (2013)
40. A.K. Grünwald, Ueber 'begrenzte' Derivationen und deren Anwendung. *Z. angew. Math. und Phys.* **12**, 441–480 (1867)
41. B. Guo, X. Pu, F. Huang, *Fractional Partial Differential Equations and their Numerical Solutions* (World Scientific, Singapore, 2011)
42. A. Hanyga, Wave propagation in media with singular memory. *Math. Comput. Modell.* **34**, 1399–1421 (2001)
43. H.J. Haubold, A.M. Mathai, R.K. Saxena, Mittag-Leffler functions and their applications. *J. Appl. Math.* **2011**, 298628 (2011). <https://doi.org/10.1155/2011/298628>
44. R. Hilfer, *Applications of Fractional Calculus in Physics* (World Scientific Publishing, River Edge, 2000)
45. R. Hilfer, H.J. Seybold, Computation of the generalized Mittag-Leffler function and its inverse in the complex plane. *Integral Transf. Spec. Funct.* **17**, 637–652 (2006)
46. J. Hristov, Diffusion models with weakly singular kernels in the fading memories: how the integral-balance method can be applied? *Thermal Sci.* **19**, 947–957 (2015)
47. C. Ingo, T.R. Barrick, A.G. Webb, I. Ronen, Accurate Padé global approximation for the Mittag-Leffler functions, its inverse, and its partial derivatives to efficiently compute convergent power series. *Int. J. Appl. Comput. Math.* 16 p. (2016). <https://doi.org/10.1007/s40819-016-0158-7>
48. C. Ionescu, J.T. Machado, R. De Keyser, J. Decruyenaere, M.M.R.F. Struys, Nonlinear dynamics of the patients response to drug effect during general anesthesia. *Commun. Nonlinear Sci. Numerical Simul.* **20**, 914–926 (2015)
49. H. Jafari, H. Tajadodi, S.A. Matikolai, Homotopy perturbation pade technique for solving fractional Riccati differential equations. *Int. J. Nonlinear Sci. Numer. Simul.* **11**, 271–276 (2010)
50. U.N. Katugampola, New approach to a generalized fractional integral. *Appl. Math. Comput.* **218**, 860–865 (2011)
51. A.A. Kilbas, M. Saigo, Generalized Mittag-Leffler function and generalized fractional calculus operators. *Integral Transf. Spec. Funct.* **15**, 31–49 (2004)
52. A.A. Kilbas, H.M. Srivastava, J.J. Trujillo, *Theory and Applications of Fractional Differential Equations* (Elsevier, Netherlands, 2006)
53. V.S. Kiryakova, Multiple (multiindex) Mittag-Leffler functions and relations to generalized fractional calculus. *J. Comput. Appl. Math.* **118**, 241–259 (2000)
54. M. Klimek, Lagrangian fractional mechanics—a noncommutative approach. *Czechoslovak J. Phys.* **55**, 1447–1453 (2005)
55. M. Klimek, *On Solutions of Linear Fractional Differential Equations of a Variational type* (The Publishing Office of Czestochowa University of Technology, Czestochowa, 2009)
56. K. Kumar, R.K. Pandey, S. Sharma, Comparative study of three numerical schemes for fractional integro-differential equations. *J. Comput. Appl. Math.* **315**, 287–302 (2017)
57. K. Kumar, R.K. Pandey, S. Sharma, Approximations of fractional integrals and Caputo derivatives with application in solving Abel's integral equations. *J. King Saud Univ. Sc.* (2018). <https://doi.org/10.1016/j.jksus.2017.12.017>
58. K.R. Lang, *Astrophysical Formulae, in Space, Time, Matter and Cosmology*, 2 (Springer, New York, USA, 1999)
59. H. Laurent, Sur le calcul des dérivées à indices quelconques. *Nouvelles Annales de Mathématiques* **3**, 240–252 (1884)
60. H. Laurent, Sur le calcul des dérivées à indices quelconques. *Nouvelles Annales de Mathématiques* **3**, 240–252 (1884)

61. J.L. Lavoie, T.J. Osler, R. Tremblay, Fractional derivatives and special functions. *SIAM Rev.* **18**, 240–268 (1976)
62. A.V. Letnikov, Theory of differentiation with an arbitrary index (Russian). *Moscow Matem. Sbornik* **3**, 1–66 (1868)
63. A.V. Letnikov, Theory of differentiation with an arbitrary index (Russian). *Moscow Matem. Sbornik* **3**, 1–66 (1868)
64. A.V. Letnikov, An explanation of the concepts of the theory of differentiation of arbitrary index (Russian). *Moscow Matem. Sbornik* **6**, 413–445 (1872)
65. C. Li, W.H. Deng, L.J. Zhao, Well-posedness and numerical algorithm for the tempered fractional ordinary differential equations. [arXiv:1501.00376v1](https://arxiv.org/abs/1501.00376v1) (2015)
66. C. Li, D. Qian, Y. Q. Chen, On Riemann–Liouville and Caputo derivatives. *Discrete Dyn. Nature Soc.* **2011** Article ID 562494, 15 p. (2011). <https://doi.org/10.1155/2011/562494>
67. J. Liouville, Mémoire sur le calcul des différentielles à indices quelconques. *J. l’Ecole Roy. Polytechn.* **13**, 71–162 (1832)
68. C.P. Li, W.H. Deng, Remarks on fractional derivatives. *Appl. Math. Comput.* **187**, 777–784 (2007)
69. C. Li, W. Deng, High order schemes for the tempered fractional diffusion equations. *Adv. Comput. Math.* **42**, 543–572 (2016)
70. J. Liouville, Mémoire sur le calcul des différentielles à indices quelconques. *J. l’Ecole Roy. Polytechn.* **13**, 71–162 (1832)
71. J. Liouville, Mémoire sur quelques questions de géométrie et de mécanique, et sur un nouveau genre de calcul pour résoudre ces questions. *J. l’Ecole Roy. Polytechn.* **13**, 1–69 (1832)
72. J. Liouville, Mémoire sur l’intégration des équations différentielles à indices fractionnaires. *J. l’Ecole Roy. Polytechn.* **15**, 58–84 (1837)
73. Y. Liu, Z. Fang, H. Li, S. He, A mixed finite element method for a time-fractional fourth-order partial differential equation. *Appl. Math. Comput.* **243**, 703–717 (2014)
74. C.F. Lorenzo, T.T. Hartley, Variable order and distributed order fractional operators. *Nonlinear Dyn.* **29**, 57–98 (2002)
75. J. Losada, J.J. Nieto, Properties of the new fractional derivative without singular kernel. *Progress Fract. Differ. Appl.* **1**, 87–92 (2015)
76. S. Ma, Y. Xu, W. Yue, Numerical solutions of a variable-order fractional financial system. *J. Appl. Math.* **2012**, Article ID 417942, 14 pp (2012). <https://doi.org/10.1155/2012/417942>
77. J.T. Machado, V. Kiryakova, F. Mainardi, Recent history of fractional calculus. *Commun. Nonlinear Sci. Numer. Simul.* **16**, 1140–1153 (2011)
78. R.L. Magin, *Fractional Calculus in Bioengineering* (Begell House Publishers, Danbury, CT, 2006)
79. F. Mainardi, R. Gorenflo, On Mittag-Leffler-type functions in fractional evolution processes. *J. Comput. Appl. Math.* **118**, 283–299 (2000)
80. A.B. Malinowska, T. Odziejewicz, D.F.M. Torres, *Advanced Methods in the Fractional Calculus of Variations* (SpringerBriefs in Applied Sciences and Technology, New York, 2015)
81. R. Maranon, J.F. Reckelhoff, Sex and gender differences in control of blood pressure. *Clin. Sci.* **125**, 311–318 (2013)
82. A. Marchaud, Sur les dérivées et sur les différences des fonctions des variables réelles. *Journal de Mathématiques Pures et Appliquées* **6**, 371–382 (1927)
83. O. Marom, E. Momoniat, A comparison of numerical solutions of fractional diffusion models in & Finance. *Nonlinear Anal.: Real World Appl.* **10**, 3435–3442 (2009)
84. M.M. Meerschaert, A. Sikorskii, *Stochastic Models for Fractional Calculus*, vol. 43 (De Gruyter, Berlin, 2012)
85. M.M. Meerschaert, Y. Zhang, B. Baeumer, Tempered anomalous diffusion in heterogeneous systems. *Geophys. Res. Lett.* **35**, L17403 (2008)
86. M.M. Meerschaert, F. Sabzikar, M.S. Phanikumar, A. Zeleke, Tempered fractional time series model for turbulence in geophysical flows. *J. Stat. Mech. Theory Exp.* **14**, 1742–5468 (2014)
87. R. Metzler, J.H. Jeon, A.G. Cherstvy, E. Barkai, Anomalous diffusion models and their properties: non-stationarity, non-ergodicity, and ageing at the centenary of single particle tracking. *Phys. Chem. Chem. Phys.* **16**, 24128–24164 (2014)

88. K.S. Miller, B. Ross, *An Introduction to the Fractional Calculus and Fractional Differential Equations* (Wiley, New York, NY, USA, 1993)
89. G. Mittag-Leffler, Sur la représentation analytique d'une branche uniforme d'une fonction monogène. *Acta Math.* **29**, 101–181 (1905)
90. T. Odziejewicz, A. B. Malinowska, D.F.M. Torres, Variable order fractional variational calculus for double integrals, 51<sup>st</sup> *IEEE Conference on Decision and Control*, December 10–13, 2012, Maui, Hawaii, art. no. 6426489, 6873–6878. <https://doi.org/10.1109/CDC.2012.6426489>
91. T. Odziejewicz, A.B. Malinowska, D.F.M. Torres, Noether's theorem for fractional variational problems of variable order. *Central Eur. J. Phys.* **11**, 691–701 (2013). <https://doi.org/10.2478/s11534-013-0208-2>
92. T. Odziejewicz, A.B. Malinowska, D.F.M. Torres, Fractional variational calculus of variable order. *Adv. Harmon. Anal. Oper. Theory* **229**, 291–301 (2013)
93. K.B. Oldham, J. Spanier, *The Fractional Calculus: Theory and Application of Differentiation and Integration to Arbitrary Order* (Academic Press, New York, NY, USA, 1974)
94. M.D. Ortigueira, *Fractional Calculus for Scientists and Engineers* (Springer, New York, 2011)
95. M.D. Ortigueira, J.A.T. Machado, Fractional signal processing and applications. *Signal Process.* **83**, 2285–2286 (2003)
96. K.M. Owolabi, A. Atangana, Numerical solution of nonlinear system in Subdiffusive, diffusive and superdiffusive scenarios. *J. Comput. Nonlinear Dyn.* **12** 031010, 7 p. (2017). <https://doi.org/10.1115/1.4035195>
97. K.M. Owolabi, Mathematical analysis and numerical simulation of patterns in fractional and classical reaction-diffusion systems. *Chaos Solitons and Fractals* **93**, 89–98 (2016)
98. K.M. Owolabi, A. Atangana, Numerical solution of fractional-in-space nonlinear Schrödinger equation with the Riesz fractional derivative. *Eur. Phys. J. Plus* **131**, 335 (2016). <https://doi.org/10.1140/epjp/i2016-16335-8>
99. I. Petras, *Fractional-Order Nonlinear Systems: Modeling Analysis and Simulation* (Springer, Berlin, 2011)
100. partial fractional differential equations, I. Podlubny, A. Chechkin, T. Skovranek, Y. Chen and B. M. Vinagre Jara, Matrix approach to discrete fractional calculus II. *J. Comput. Phys.* **228**, 3137–3153 (2009)
101. I. Podlubny, *Fractional Differential Equations* (Academic Press, San Diego, 1999)
102. H. Qi, X. Guo, Transient fractional heat conduction with generalized Cattaneo model. *Int. J. Heat Mass Transf.* **76**, 535–539 (2014)
103. L.E.S. Ramirez, C.F.M. Coimbra, On the selection and meaning of variable order operators for dynamic modeling. *Int. J. Differ. Equ.* (846107), 16 (2010)
104. L.E.S. Ramirez, C.F.M. Coimbra, On the variable order dynamics of the nonlinear wake caused by a sedimenting particle. *Physica D* **240**, 1111–1118 (2011)
105. M. Riesz, L'intégrales de Riemann-Liouville et le problème de Cauchy. *Acta Math.* **81**, 1–223 (1949)
106. M. Riesz, L'intégrales de Riemann-Liouville et solution invariante du problème de Cauchy pour l'équation des ondes. *C. R. Congrès Intern. Math.* **2**, 44–45 (1936)
107. M. Riesz, L'intégrales de Riemann-Liouville et le problème de Cauchy. *Acta Math.* **81**, 1–223 (1949)
108. F. Sabzikar, M.M. Meerschaert, J. Chen, Tempered fractional calculus. *J. Comput. Phys.* **292**, 14–28 (2015)
109. S.G. Samko, B. Ross, Integration and differentiation to a variable fractional order. *Integral Transf. Spec. Funct.* **1**, 277–300 (1993)
110. S. Samko, A. Kilbas, O. Marichev, *Fractional Integrals and derivatives: Theory and Applications* (Gordon and Breach, Amsterdam, 1993)
111. W.E. Schiesser, *Numerical Method of Lines Integration of Partial Differential Equations* (Academic Press, San Diego, 1991)
112. N.Y. Sonin, On differentiation with arbitrary index. *Moscow Matem. Sbornik* **6**, 1–38 (1869)
113. H.G. Sun, X. Hao, Y. Zhang, D. Baleanu, Fractional derivative defined by non-singular kernels to capture anomalous relaxation and diffusion. [arXiv:1606.04844v2](https://arxiv.org/abs/1606.04844v2) [cond-mat.stat-mech] (2016)

114. H.G. Sun, W. Chen, C.P. Li, Y.Q. Chen, Fractional differential models for anomalous diffusion. *Physica A* **389**, 2719–2724 (2010)
115. N. Tatar, The decay rate for a fractional differential equation. *J. Math. Anal. Appl.* **295**, 303–314 (2004)
116. D. Tavares, R. Almeida, D.F.M. Torres, Caputo derivatives of fractional variable order: numerical approximations. *Commun. Nonlinear Sci. Numer. Simul.* **35**, 69–87 (2016)
117. L. Turgeman, S. Carmi, E. Barkai, Fractional Feynman-Kac equation for non-Brownian functionals. *Phys. Rev. Lett.* **103**, 190201 (2009)
118. V.V. Uchaikin, *Fractional Derivatives for Physicists and Engineers* (Higher Education Press and Springer Verlag, Beijing/Berlin, Background and Theory, 2013)
119. H. Vandebroek, C. Vanderzande, Transient behaviour of a polymer dragged through a viscoelastic medium. *J. Chem. Phys.* **141**, 114910 (2014)
120. Y. Watanabe, Notes on the generalized derivative of Riemann–Liouville and its application to Leibnitz’s formula. I and II, *Tohoku Math. J.* **34**, 8–41 (1931)
121. H. Weyl, Bemerkungen zum Begriff des differential quotienten gebrochener Ordnung. *Vierteljahrsh. Naturforsch. Gesellsch. Zürich* **62**, 296–302 (1917)
122. H. Weyl, Bemerkungen zum Begriff des Differential quotienten gebrochener Ordnung. *Vierteljahrsh. Naturforsch. Gesellsch. Zürich* **62**, 296–302 (1917)
123. S. Yadav, R.K. Pandey, A.K. Shukla, Numerical approximations of Atangana-Baleanu Caputo derivative and its application. *Chaos, Solitons and Fractals* **118**, 58–64 (2019)
124. G.M. Zaslavsky, *Hamiltonian Chaos and Fractional Dynamics* (Oxford University Press, New York, 2005)
125. S. Zhang, Y. Yu, H. Wang, Mittag–Leffler stability of fractional-order Hopfield neural networks. *Nonlinear Anal.: Hybrid Syst.* **16**, 104–121 (2014)
126. Y.Y. Zheng, C.P. Li, Z. G. Zhao, A fully discrete discontinuous Galerkin method for nonlinear fractional fokker-planck equation. *Math. Problems Eng.* **2010**, Article ID 279038, 26 p. (2010)
127. B. Zheng,  $(G'/G)$ -expansion method for solving fractional partial differential equations in the theory of mathematical physics. *Commun. Theor. Phys.* **58**, 623–630 (2012)
128. P. Zhuang, F. Liu, V. Anh, I. Turner, New solution and analytical techniques of the implicit numerical method for the anomalous subdiffusion equation. *SIAM J. Numer. Anal.* **46**, 1079–1095 (2008)

## Chapter 2

# Finite Difference Approximations



This chapter presents the formulation of higher order finite difference (FD) formulas for the spatial approximation of the time-dependent reaction–diffusion problems with a clear justification through examples, the supremacy between the second- and fourth-order schemes. As a consequence, methods for the solution of initial and boundary value PDEs, such as the method of lines (MOL), is of broad interest in science and engineering. This procedure begins with the discretization of the spatial derivatives in the PDE with algebraic approximations. The key idea of MOL is to replace the spatial derivatives in the PDE with the algebraic approximations. Once this procedure is done, the spatial derivatives are no longer stated explicitly in terms of the spatial independent variables. In other words, only one independent variable is remaining, the resulting semi-discrete problem has now become a system of coupled ordinary differential equations (ODEs) in time. Thus, one can apply any integration algorithm for the initial value ODEs to compute an approximate numerical solution to the PDE. Analysis of the basic properties of these schemes such as the order of accuracy, convergence, consistency, stability and symmetry are well examined in this chapter.

Reaction–diffusion equations are classified as a special class of parabolic time-dependent partial differential equations. The major way of solving the class of these equations is through discretization. A well-known approach to solve time-dependent partial differential equation, whose solutions vary both in time and space, is the *method of lines* (MOL), Schisser and Griffiths [35] and Stricwerda [40]. Application of this method requires to first construct a semi-discrete approximation to the problem by setting up a regular grid in space, this is achieved by discretizing the spatial independent variables with boundary constraints. Hence, a couple system of ordinary differential equations are generated in time, which is associated with the initial value. Once that is done, we numerically approximate the solutions to the original time-dependent partial differential equation by marching forward in time on this grid.

Conveniently, we can now apply any existing, and generally well established, time-stepping numerical methods such as the implicit–explicit (IMEX) schemes, Runge–Kutta methods or exponential time differencing (ETD) schemes among many others.

In this chapter, for the spatial discretization, we are primarily concerned with the use of higher order finite difference method. The discrete approximation to the derivatives will be converted into Toeplitz matrices. The discretization in time uses majorly the exponential time differencing schemes, other time-stepping methods include but not limited to the fourth-order Runge–Kutta (RK4) method and implicit–explicit schemes. A brief of each of these methods will be discussed later in this chapter. Once computational experiments are conducted, there are some important issues such as consistency, stability and convergence that are required to be investigated, the moment these issues as pointed out are addressed, we can now proceed to solve numerically to solve all the classes of reaction–diffusion problems to be considered.

## 2.1 Finite Difference Approximation Schemes

As one briefly learns, the differential equations that can be solved by explicit analytic formulae are few and far between. Consequently, the development of accurate numerical approximation schemes is essential for extracting quantitative information as well as achieving a qualitative understanding of the various behaviours of their solutions. Even in cases, such as the heat and wave equations, where explicit solution formulas (either closed-form or infinite series) exist, numerical methods can still be profitably employed. Indeed, one can accurately test a proposed numerical algorithm by running it on a known solution, providing yet another motivation to search for explicit solutions. An alternative approach is to use a manufactured solution, in which one starts with a preselected function, which almost certainly is not a solution to the problem at hand.

Nevertheless, substituting this function into the differential equation and the relevant initial and boundary conditions lead to an inhomogeneous problem of the same character as the original. After running the numerical algorithm on the modified problem, one can test for accuracy by comparing the numerical output with the preselected function. The lessons learned in the design and testing of numerical algorithms for simpler solved example, for instance, the diffusion equation is of inestimable value when confronting more challenging reaction–diffusion problems. Many of the basic numerical solution schemes for partial differential equations can be fit into two broad themes. The first, to be developed in the present chapter, are the finite difference methods, obtained by replacing the derivatives in the equation by appropriate numerical differentiation formulae.

We thus start with a brief discussion of some elementary finite difference formulae used to numerically approximate first and second-order derivatives of functions as we are going to see the details in under the numerical experiments. As a basic, since most or almost reaction–diffusion problems proposed for consideration in this thesis have

the heat or diffusion equation as the basis, we then establish and analyse some of the most basic finite difference schemes for the heat or diffusion equation. As we will also learn, not all finite difference approximations lead to accurate numerical schemes, and one must deal with the issues of stability and convergence in order to distinguish reliable from worthless methods. In fact, we are inspired by Fourier analysis, the crucial stability criterion follows from how the numerical scheme handles basic complex exponentials.

The finite difference methods have gained dominance in the various fields of computational science since its inception as the major method of choice back to 1960s. Other methods such as finite element and boundary element methods enjoyed recent popularity, finite difference methods are still well utilized for a wide array of computational engineering and science problems.

A finite difference scheme is produced when the partial derivatives in the partial differential equation(s) governing a physical phenomenon are replaced by a finite difference approximation. The result is a single algebraic equation or a system of algebraic equations which, when solved, provide an approximation to the solution of the original partial differential equation at selected points of a solution grid. The solution grid (also referred to as computational grid or numerical grid) is originated by dividing the axes representing the independent variables in the solution domain into a number of intervals. The extreme points of the interval will represent points in the solution grid. If we draw lines perpendicular to given axes passing through the extreme points of the intervals, the resulting grid is the computational grid.

### 2.1.1 Taylor Series and Finite Difference Approximation

In the study of elementary calculus, the standard definition of derivative is of the form

$$u'(x) = \lim_{\Delta x \rightarrow 0} \frac{u(x + \Delta x) - u(x)}{\Delta x}; \quad (2.1.1)$$

it is clear that computer cannot deal with the  $\Delta x \rightarrow 0$ , so there to adopt a discrete analogue of the continuous function. We shall use the notation  $u_j = u(x_j)$  to denote the value of the function at the  $j$ -th node of the computational grid. The nodes divide the axis into a set of intervals of width  $\Delta x_j = x_{j+1} - x_j$ , for a fixed space, we expect the intervals to be of equal size which we shall denote here as  $\Delta x$ .

It would probably be a good notion to briefly review some facts surrounding the Taylor's series before proceeding to discuss the mathematical formalities of the finite difference formulas perse. From the concept of elementary calculus, we know that the Taylor series method is used to find the expansion of a function, say, for instance,  $u(x)$  as a power series,

$$u(x) = u(a) + \frac{(x-a)}{1!}u'(a) + \frac{(x-a)^2}{2!}u''(a) + \dots = \sum_{k=0}^{\infty} \frac{(x-a)^k}{k!}u^{(k)}(a). \quad (2.1.2)$$

In this context, we shall replace  $x$  and  $a$  by  $x_j + \Delta x$  and  $x_j$ , respectively. We would refer to  $\Delta x$  as the increment in  $x$ . Hence, we can now write the Taylor series in the form

$$u(x_j + \Delta x) = u(x_j) + \frac{(\Delta x)}{1!}u'(x_j) + \frac{(\Delta x)^2}{2!}u''(x_j) + \dots = \sum_{k=0}^{\infty} \frac{(\Delta x)^k}{k!}u^{(k)}(x_j). \quad (2.1.3)$$

and

$$u(x_j - \Delta x) = u(x_j) - \frac{(\Delta x)}{1!}u'(x_j) + \frac{(\Delta x)^2}{2!}u''(x_j) - \dots = \sum_{k=0}^{\infty} (-1)^k \frac{(\Delta x)^k}{k!}u^{(k)}(x_j). \quad (2.1.4)$$

The definition of the derivative in the continuum can be used to approximate the derivative in the discrete case. For the treatment of many problems, it is much more convenient to take only the first two terms of the right-hand side of (2.1.3), now we have

$$u(x_j + \Delta x) = u(x_j) + \Delta x u'(x_j) + \mathcal{O}(\Delta x), \quad (2.1.5)$$

where the expression  $\mathcal{O}(\Delta x)$  denotes the truncation error arising from truncating the Taylor series approximation that is proportional to  $\Delta x$ . Using relationship (2.1.5), we can obtain the **first-order forward difference approximation** to  $u'(x)$  as

$$u'(x)|_{x=x_j} = \frac{u(x_j + \Delta x) - u(x_j)}{\Delta x} + \mathcal{O}(\Delta x), \quad (2.1.6)$$

and on replacing  $\Delta x$  by  $-\Delta x$ , we have

$$u'(x)|_{x=x_j} = \frac{u(x_j) - u(x_j - \Delta x)}{\Delta x} + \mathcal{O}(\Delta x), \quad (2.1.7)$$

which is referred to as the **first-order backward difference approximation** to  $u'(x)$ .

By subtracting Eq. (2.1.4) from Eq. (2.1.3), we obtain

$$u(x_j + \Delta x) - u(x_j - \Delta x) = 2\Delta x u'(x_j) + \mathcal{O}(\Delta x^3),$$

which when rearranged yields

$$u'(x_j) = \frac{u(x_j + \Delta x) - u(x_j - \Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^2). \quad (2.1.8)$$

Equation (2.1.8) is referred to as the **second-order centred difference approximation** for  $u'(x)$  at point  $x = x_j$ .

Again, upon adding Eqs. (2.1.3) and (2.1.4),

$$u(x_j + \Delta x) - u(x_j - \Delta x) = 2u(x_j) + (\Delta x)^2 u''(x_j) + \mathcal{O}(\Delta x^4),$$

which we rearrange to have

$$u''(x_j) = \frac{u(x_j + \Delta x) - 2u(x_j) + u(x_j - \Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2) \quad (2.1.9)$$

known as the **second-order central difference approximation** to  $u''(x)$ . The right-hand side of Eq. (2.1.9) is the error committed in terminating the series and is referred to as the truncation error. The truncation error can be defined as the difference between the partial derivative and its finite difference representation.

### 2.1.2 Higher Order Finite Difference Approximation

Higher order finite difference approximations can be obtained by taking more terms in Taylor series expansion. The Taylor expansion provides a very useful tool for the derivation of higher order approximation to derivatives of any order. Our interest in this work is to use higher order finite difference formula for the spatial discretization of the problems to be considered later in this work, so we need to create an estimate based on step size  $2\Delta x$  through the Taylor series expansion

$$u(x_j + 2\Delta x) = \sum_{k=0}^{\infty} \frac{(2\Delta x)^k}{k!} u^{(k)}(x_j) \quad (2.1.10)$$

$$u(x_j - 2\Delta x) = \sum_{k=0}^{\infty} (-1)^k \frac{(2\Delta x)^k}{k!} u^{(k)}(x_j). \quad (2.1.11)$$

Better approximation is obtained by combining these two estimates through the process called Richardson extrapolation. For instance, we present the fourth-order centred finite difference schemes for the first and second derivatives as

$$u'(x_j) = \frac{u(x_j - 2\Delta x) - 8u(x_j - \Delta x) + 8u(x_j + \Delta x) - u(x_j + 2\Delta x)}{12\Delta x} + \mathcal{O}(\Delta x)^4 \quad (2.1.12)$$

and

$$u''(x_j) = \frac{-u(x_j - 2\Delta x) + 16u(x_j - \Delta x) - 30u(x_j) + 16u(x_j + \Delta x) - u(x_j + 2\Delta x)}{12\Delta x^2} + \mathcal{O}(\Delta x)^4 \quad (2.1.13)$$

**Table 2.1** Weights of some higher order centred finite difference approximation for the first derivative on equi-spaced grids

Order of accuracy	$u_{-4}$	$u_{-3}$	$u_{-2}$	$u_{-1}$	$u_0$	$u_1$	$u_2$	$u_3$	$u_4$
2				$-\frac{1}{2}$	0	$\frac{1}{2}$			
4			$-\frac{1}{12}$	$-\frac{8}{12}$	0	$\frac{8}{12}$	$-\frac{1}{12}$		
6		$-\frac{1}{60}$	$\frac{9}{60}$	$-\frac{45}{60}$	0	$\frac{45}{60}$	$-\frac{9}{60}$	$\frac{1}{60}$	
8	$\frac{3}{840}$	$-\frac{32}{840}$	$\frac{168}{840}$	$-\frac{672}{840}$	0	$\frac{672}{840}$	$-\frac{168}{840}$	$\frac{32}{840}$	$-\frac{3}{840}$

**Table 2.2** Weights of some higher order centred finite difference approximation for the second derivative on equi-spaced grids

Order of accuracy	$u_{-4}$	$u_{-3}$	$u_{-2}$	$u_{-1}$	$u_0$	$u_1$	$u_2$	$u_3$	$u_4$
2				1	-2	1			
4			$-\frac{1}{12}$	$\frac{16}{12}$	$-\frac{30}{12}$	$\frac{16}{12}$	$-\frac{1}{12}$		
6		$\frac{2}{180}$	$-\frac{27}{180}$	$\frac{270}{180}$	$-\frac{490}{180}$	$\frac{270}{180}$	$-\frac{27}{180}$	$\frac{2}{180}$	
8	$-\frac{1}{560}$	$\frac{8}{315}$	$-\frac{1}{5}$	$\frac{8}{5}$	$-\frac{205}{72}$	$\frac{8}{5}$	$-\frac{1}{5}$	$\frac{8}{315}$	$-\frac{1}{560}$

respectively. For the purpose of comparison, we present the conventional second-order FD scheme as

$$u''(x_j) = \frac{u(x_j + \Delta x) - 2u(x_j) + u(x_j - \Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2). \tag{2.1.14}$$

Some of the important features to notice about centred finite difference schemes, they are symmetric in nature and possess an even order of accuracy. The weights of some of the central finite difference formulas are presented in the following tables for the approximations of first and second derivatives.

where  $u_i$  for  $i = 1, 2, 3, 4$  has the following equivalence in the tables:

$$\begin{aligned}
 u_{-4} &\equiv u(x_j - 4\Delta x) \\
 u_{-3} &\equiv u(x_j - 3\Delta x) \\
 &\vdots \\
 u_o &\equiv u(x_j) \\
 &\vdots \\
 u_3 &\equiv u(x_j + 3\Delta x) \\
 u_4 &\equiv u(x_j + 4\Delta x).
 \end{aligned}$$

In general, schemes for any given derivatives of any chosen order can be derived from Taylor expansions as long as sufficient number of sample points are used.

These approximations are much more difficult far beyond the simple cases shown, most especially, the higher order formulas. Readers are referred to the books by Fornberg [8], Fornberg and Driscoll [10] where schematic illustration of how to generate the weights of higher order centred and one-side finite differences formulas for approximating derivatives up to fourth-order equi-spaced grids with order of accuracy up to eighth can be found.

For more general finite difference approximations, we follow the description given by Fornberg [9] and present briefly the short code that can be used to generate weights of any order approximation schemes on an equi-spaced grid. The program only requires **Mathematica**<sup>®</sup> (version seven and above) that is contained pre-loaded Padé package. The complete code is

```
t = PadeApproximation [xs(Log[x]/h)m, {x, 1, {n, d}}];
CoefficientList [{Denominator[t], Numerator[t]}, x].
```

The numbers  $d$ ,  $m$ ,  $n$  and  $s$  describe the shape of the stencil, where  $d$  is the number of grid intervals in between the left- and rightmost derivative entries,  $m$  indicates the number of derivatives to be approximated,  $n$  stands for the number of grid intervals in between the left- and rightmost function entries, and  $s$  the number of grid intervals in between the leftmost derivative and function entries.

## 2.2 Error Analysis

Next, we need to ask ourselves why using fourth-order approximation scheme instead of the commonly used second-order scheme approximation? To answer this question, let us quickly consider an example. Given  $u(x) = \cos(x)$ , let us use formulas (2.1.14) and (2.1.13) with  $\Delta x = 0.1$ , 0.01 and 0.001 to find approximations to  $u''(0.8)$ . The true value here is taken to be  $u''(0.8) = -\cos(0.8)$ . For instance, the calculation for  $\delta x = 0.01$  with methods (2.1.14) is

$$\begin{aligned} u''(0.8) &\approx \frac{u(0.81) - 2u(0.80) + u(0.79)}{0.0001} \\ &\approx \frac{0.689498433 - 2(0.696706709) + 0.703845316}{0.0001} \\ &\approx -0.696690000. \end{aligned}$$

By subtracting the computed value from the true value, we found the error in this approximation to be  $1.0671e - 005$ . The remaining calculations are summarized in Table 2.3.

In the same manner, we present the results of approximations fourth-order formula (2.1.13).

**Table 2.3** Numerical approximations using second-order formula (2.1.14)

Step size ( $\Delta x$ )	Approximation	Error
$\Delta x = 1.0$	-0.640548935	-0.056157774
$\Delta x = 0.1$	-0.696126300	-0.000580409
$\Delta x = 0.01$	-0.696690000	-0.000016709
$\Delta x = 0.001$	-0.696000000	-0.000706709

**Table 2.4** Numerical approximations using fourth-order formula (2.1.13)

Step size ( $\Delta x$ )	Approximation	Error
$\Delta x = 1.0$	-0.689625413	-0.007081296
$\Delta x = 0.1$	-0.696705958	-0.000000751
$\Delta x = 0.01$	-0.696000000	-0.000016709
$\Delta x = 0.001$	-0.696675000	-0.000031709

The results obtained in Tables 2.3 and 2.4 have shown that the fourth-order scheme produces a better approximation when compared to its second-order counterpart. The optimal step size for the formula (2.1.14) is at when  $\Delta x = 0.01$  as shown in Table 2.3 and the optimal step size to be used for Eq. (2.1.13) is when  $\Delta x = 0.1$ . We can see here that the fourth-order allows large step size.

We need to analyse briefly the two approximation methods of orders  $\mathcal{O}(\Delta x^2)$  and  $\mathcal{O}(\Delta x^4)$  that are paramount to our discussion. Let  $u_k = \zeta_k + \epsilon_k$ , where  $\epsilon_k$  is the error in computing  $u(x_k)$ , we can write the second-order approximation formula (2.1.14) in the form

$$u''(x) = \frac{u(x + \Delta x) - 2u(x) + u(x - \Delta x)}{\Delta x^2} + E(u, \Delta x). \tag{2.2.1}$$

The error term  $E(u, \Delta x)$  consists of both truncation error and the round-off error. That is,

$$\begin{aligned} E(u, \Delta x) &= E_{round}(u, \Delta x) + E_{trunc}(u, \Delta x) \\ &= \frac{\epsilon(x + \Delta x) - 2\epsilon(x) + \epsilon(x - \Delta x)}{\Delta x^2} - \frac{\Delta x^2 u^{(4)}(c)}{12}, \end{aligned} \tag{2.2.2}$$

where  $|u^{(4)}(c)|$  is supposed to be bounded for  $c = c(x) \in [x - \Delta x, x + \Delta x]$ , then the truncation error in (2.2.2) goes to zero in the same manner as  $\Delta x^2$  which is expressed with notation  $\mathcal{O}(\Delta x^2)$  in (2.1.14). Since it is assumed that each error  $\epsilon_k$  has magnitude  $\xi$ , and that  $|u^{(4)}(x)| \leq M$ , then we can obtain the error bound, if  $|\epsilon_k| \leq \xi$  and  $M = \max [x - \Delta x, x + \Delta x] \{u^{(4)}(x)\}$ , then

$$|E(u, \Delta x)| \leq \frac{4\xi}{\Delta x^2} + \frac{M\Delta x^2}{12}. \tag{2.2.3}$$

A small value of  $\Delta x$  will make  $4\xi/\Delta x^2$  coming from the round-off error to be large. Also, when  $\Delta x$  is large, the contribution  $M\Delta x^2/12$  is large as well. So, the optimum step size will minimize the quantity

$$\gamma(\Delta x) = \frac{4\xi}{\Delta x^2} + \frac{M\Delta x^2}{12}, \quad (2.2.4)$$

with  $\gamma'(\Delta x) = 0$ , we obtain

$$-\frac{8\xi}{\Delta x^3} + \frac{M\Delta x^2}{6} = 0$$

which when simplifying further yields

$$\Delta x^2 = \frac{48\xi}{M},$$

from which optimal value is obtained as

$$\Delta x = \left(\frac{48\xi}{M}\right)^{\frac{1}{4}}, \quad (2.2.5)$$

and that

$$M = |u^{(4)}(x)| \leq |\cos(x)| \leq 1.$$

It is clear that the portion of the error due to round-off is inversely proportional to the square of  $\delta x$ , this particular term grows when  $\Delta x$  gets small, and it is referred to as the step-size dilemma in most cases. The only way out of this problem is to use a higher order method that would accommodate a larger value of  $\Delta x$  to yield the desired accuracy. This assertion actually prompts us to seek higher order approximation method.

Considering (2.1.13), the error term has the form

$$E(u, \Delta x) = \frac{16\xi}{3\Delta x^2} + \frac{\Delta x^4 u^{(6)}(c)}{90}, \quad (2.2.6)$$

where  $c$  lies in the interval  $[x - 2\Delta x, x + \Delta x]$ . We define a bound for  $|E(u, \Delta x)|$  as

$$|E(u, \Delta x)| \leq \frac{16\xi}{3\Delta x^2} + \frac{\Delta x^4 M}{90}, \quad (2.2.7)$$

with  $|u^{(6)}(x)| \leq M$ . Thus, the optimal value for  $\Delta x$  is given by

$$\Delta x = \left( \frac{240\xi}{M} \right)^{\frac{1}{6}}, \quad (2.2.8)$$

and that

$$M = |u^{(6)}(x)| \leq |\cos(x)| \leq 1$$

### 2.2.1 Illustrative Example

Most physical applications in the world today are generally described in scientific and engineering terms with respect to dimensions in both space and time. Most mathematical descriptions exist in terms of partial differential equations explaining the concept of physical space–time. As a result of this fact, methods for the solution of partial differential equations, such as the method of lines by Hamdi et al. [13] and Strikwerda [40] are still active in the current field of research. As a basic illustrative example of a PDE, let us consider the diffusion equation

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, \quad a \leq x \leq N, \quad t_{init} \leq t \leq t_{final}, \quad (2.2.9)$$

where  $u$  is the dependent variable that depends on independent variables  $x$  and  $t$  representing the one-dimensional and time, respectively. The presence of two independent variables in (2.2.9) is the reason it is classified as a PDE. If the number of independent variables is just one, such an equation is known to be ordinary differential equation (ODE). In literature, Eq. (2.2.9) is regarded as diffusion or heat equation. When applied to heat transfer, it becomes the Fourier second law, the dependent variable  $u$  is the temperature and  $D$  is the thermal diffusivity. But in the area of mathematical biology, which is the main scope of this work, when Eq. (2.2.9) is applied to mass diffusion, it obeys Fick's second law and  $u$  is termed the concentration while  $D$  is the diffusion coefficient whose value must always be greater than zero.

Solution of equation of the form (2.2.9) is subjected to some auxiliary conditions that can be determined by the highest order of the derivatives in each of the independent variables present (see Powers [32], Meyer [25], Kreiss and Lorenz [19]). We refer to  $t$  as an initial value variable that requires an initial condition that starts at say  $t_0 = 0$  and moves over a finite interval  $t_0 \leq t \leq T$  or on semi-infinite interval  $t_0 \leq t \leq \infty$ .  $x$  is known as the boundary value variable that requires two boundary conditions to be specified at both ends. This boundary value variable is expected to be varied over a finite interval  $a \leq x \leq N$ , a semi-infinite interval  $a \leq x \leq \infty$  or over a fully infinite interval  $-\infty \leq x \leq \infty$ . So, we can write the initial condition at  $t_0 = 0$  in the form

$$u(x, t = 0) = u_0(x),$$

and the corresponding two boundary conditions could be

$$\begin{aligned}u(x = a, t) &= f_a(t) \\u(x = N, t) &= f_N(t),\end{aligned}$$

where  $f_a(t)$  and  $f_N(t)$  are the given boundary values of  $u$  for all  $t$ . The basic idea of the method of lines is to replace the spatial derivatives in the partial differential equation with algebraic approximations. On doing this, the spatial derivatives are no longer written explicitly in terms of the spatial independent variables, leaving behind only the initial variable typically time in a physical problem. Thus, with only one independent variable left, we obtain a system of ordinary differential equations that approximate the original partial differential equation. The major task remains, how to formulate the approximating system of ODEs. Once this is done, we can now employ any integration algorithm for the initial value ODEs to compute an approximate numerical solution to the PDE.

To illustrate the method of lines procedure to solve diffusion equation (2.2.9), suppose that  $u(x, t)$  is discretized in space with  $N + 1$  points, of which  $N - 1$  are the interior points, on a uniform grid with step-size  $\delta x$ , we have

$$u(x_j, t) \approx u_j(t), \quad 0 \leq j \leq N, \quad (2.2.10)$$

where the index  $j$  indicating a position along the grid in  $x$  and  $\Delta x$  is the spacing in  $x$  along the grid, assumed to be constant. To find an algebraic approximation to the spatial derivative  $\frac{\partial^2 u}{\partial x^2}$  in Eq. (2.2.9), for instance, with the fourth-order centred finite difference approximation (2.1.13) as discussed above, in such that

$$\left. \frac{\partial^2 u}{\partial x^2} \right|_{x=x_j} \approx \frac{-u_{j+2}(t) + 16u_{j+1}(t) - 30u_j(t) + 16u_{j-1}(t) - u_{j-2}(t)}{12\Delta x^2} + \mathcal{O}(\Delta x^4). \quad (2.2.11)$$

Then the method of lines approximation of Eq. (2.2.9), gives a system ODEs

$$\begin{aligned}u_0(t) &= f_a(t), \\ \frac{du_1(t)}{dt} &= D \left[ \frac{-u_4(t) + 16u_3 - 30u_2 + 16u_1(t) - u_0t}{12\Delta x^2} \right] \\ \frac{du_2(t)}{dt} &= D \left[ \frac{-u_5(t) + 16u_4 - 30u_3 + 16u_2(t) - u_1t}{12\Delta x^2} \right] \\ &\vdots \\ &\vdots \\ \frac{du_{N-1}(t)}{dt} &= D \left[ \frac{-u_N(t) + 16u_{N-1}(t) - 30u_{N-2}t + 16u_{N-3}(t) - u_{N-4}(t)}{12\Delta x^2} \right] \\ u_N(t) &= f_N(t),\end{aligned} \quad (2.2.12)$$

subject to the initial conditions

$$u_j(x, t = 0) = u_0(x_j), \quad 0 \leq j \leq N. \quad (2.2.13)$$

Equations (2.2.12) and (2.2.13) now constitute the complete method of lines approximation of Eq. (2.2.9).

### 2.2.2 Order of Accuracy and Consistency

To ascertain the order of accuracy of a scheme, the finite difference approximation has to be compared to the approximated differential. After having examined the accuracy of individual derivatives, we will now analyse the accuracy of approximation for partial differential equations. As a result of basic test case, we use the diffusion equation

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}, \quad (2.2.14)$$

with  $D > 0$ , which we used forward difference scheme in time coupled with the central difference (2.1.14) scheme in space, in such a way that Eq. (2.2.14) is transformed to

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} - D \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} = 0. \quad (2.2.15)$$

The modified equation for this scheme is now formulated at the point, say  $(x_0, t_0)$  to yield

$$\frac{u(x_0, t_0 + \Delta t) - u(x_0, t_0)}{\Delta t} - D \frac{u(x_0 + \Delta x, t_0) - 2u(x_0, t_0) + u(x_0 - \Delta x, t_0)}{\Delta x^2} = 0. \quad (2.2.16)$$

Next, the difference between the modified equation and the differential equation is then built for checking the consistency of the scheme determining its order of approximation obtained by means of a Taylor expansion, we have

$$\begin{aligned} & \frac{u(x_0, t_0 + \Delta t) - u(x_0, t_0)}{\Delta t} - D \frac{u(x_0 + \Delta x, t_0) - 2u(x_0, t_0) + u(x_0 - \Delta x, t_0)}{\Delta x^2} \\ & + \partial_t u(x_0, t_0) - D \partial_{xx} u(x_0, t_0) \\ & = -\frac{\Delta t}{2} \partial_{tt} u(x_0, t_0) + D \frac{\Delta x^2}{24} \partial_{xxxx} u(x_0, t_0) \\ & - \frac{\Delta t^2}{6} \partial_{ttt} u(x_0, t_0) + D \frac{\Delta x^4}{320} \partial_{xxxxx} u(x_0, t_0) + \dots \\ & = \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2). \end{aligned} \quad (2.2.17)$$

The right-hand side of (2.2.17) is the so-called truncation error, and the lowest powers of  $\Delta t$  and  $\Delta x$  in the truncation error are the respective order of accuracies of the finite difference approximations in time and space. Thus, the finite difference scheme

(2.2.15) is consistent with the diffusion equation (2.2.14) to first-order accuracy in time and second-order accuracy in space.

In the same way, we verify the consistency and accuracy of fourth order finite difference approximations (2.1.12) and (2.1.13) when used to discretized the diffusion equation (2.2.14). Thus, after expanding each terms in Taylors series and collect the terms in equal powers of  $\Delta t$  and  $\Delta x$ , we obtain

$$\begin{aligned}
 & \frac{-u(x_0, t_0 + 2\Delta t) + 8u(x_0, t_0 + \Delta t) - 8u(x_0, t_0 - \Delta t) + u(x_0, t_0 - 2\Delta t)}{12\Delta t} \\
 & - D \frac{-u(x_0 + 2\Delta x, t_0) + 16u(x_0 + \Delta x, t_0) - 30u(x_0, t_0) + 16u(x_0 - \Delta x, t_0)}{12\Delta x^2} \\
 & - \frac{u(x_0 - 2\Delta x, t_0)}{12\Delta x^2} + \partial_t u(x_0, t_0) + D\partial_{xx}u(x_0, t_0) \\
 & = \frac{\Delta t^4}{30}\partial_{tttt}u(x_0, t_0) + D\frac{\Delta x^4}{90}\partial_{xxxx}u(x_0, t_0) + \dots
 \end{aligned} \tag{2.2.18}$$

Since the truncation error is defined as  $T_j^n = u(x_j, t_n) - u_j^n$ . Therefore

$$|T_j^n| \leq \beta_1 \Delta t^4 + \beta_2 \Delta x^4,$$

where  $\beta_1$  and  $\beta_2$  denote two constants that depend on some norms of the derivatives of  $u$ . As a result, this scheme is consistent with order of accuracy 4 in both space and time.

Generally, if the truncation error is  $\mathcal{O}(\Delta x^p, \Delta t^q)$ , the method is  $p$ th order accurate in  $x$  and  $q$ th order accurate in  $t$ . If the truncation error tends to zero as  $\Delta x, \Delta t \rightarrow 0$ , the scheme is called *consistent*.

A finite difference method is convergent to  $p$ th order in  $x$  and  $q$ th order in  $t$  if

$$\|u(x_j, t_n) - u_j^n\| = \mathcal{O}(\Delta x^p) + \mathcal{O}(\Delta t^q) \quad \text{as } \Delta x, \Delta t \rightarrow 0 \tag{2.2.19}$$

for  $x_j, t_n < T$ , where  $T$  is some positive time independent of  $\Delta x, \Delta t$  and

$$\|u\|_p = \left( \sum_{j=1}^N |u_j|^p \Delta x \right)^{\frac{1}{p}},$$

where  $p = 2$  corresponds to Euclidean norm and  $p = \infty$  is the maximum norm.

**Definition 2.2.1** A finite difference method is

(i) Stable if

$$\|u^n\| \leq C_T \|u^0\|$$

for  $n\Delta t \leq T$ , a fixed positive time, and all sufficiently small  $\Delta x, \Delta t$ .

(ii) Exponentially stable if

$$C_T \leq Ae^{BT}$$

and

(iii) Strictly stable if  $C_T \leq 1$ .

### The Lax Equivalence Theorem

By Lax equivalence theorem (Lax and Richtmeyer [21]), the importance of the concepts of consistency and stability is seen in the Lax–Richtmyer equivalence theorem, which is the fundamental theorem in the theory of finite difference schemes for initial value problem. It states that, if a finite difference method for a given partial differential equation for which initial value problem is well posed and that the scheme is linear, stable and accurate of order  $\mathcal{O}(\Delta x^p, \Delta t^q)$ , it is convergent.

The essential idea of the Lax equivalence theorem is this: for consistent linear finite difference models, stability is a necessary and sufficient condition for convergence. This is an analogue of the Dahlquist equivalence theorem for ordinary differential equations [43]. Aside from the assumption of linearity, the formulation of the Lax equivalence theorem is very general. Let  $\mathbb{B}$  be a Banach space (a complete normed vector space) with norm denoted by  $\|\cdot\|$ . In applications of interest here each element of  $\mathbb{B}$  will be a function of one or more space variables  $x$ . Let  $A : \mathbb{B} \rightarrow \mathbb{B}$  be a linear operator on this space. Here  $A$  will be a differential operator. Assuming we are given the initial value problem

$$u_t(t) = Au(t), \quad 0 \leq t \leq T, \quad u(0) = u_0, \quad (2.2.20)$$

where  $A$  is fixed but  $u_0$  may range over all elements of  $\mathbb{B}$ . [Note,  $A$  is defined on a dense subset of  $\mathbb{B}$ .] It is assumed that the initial value problem (2.2.20) is well posed, which implies that a unique solution  $u(t)$  exists for any initial data  $u_0$  and that  $u(t)$  depends continuously upon the initial data.

**Definition 2.2.2** A numerical scheme that is symmetric is consistent [7, 20] if:

(i) It has order  $(p, q) \geq 1$ . If a scheme has order  $(p, q) \geq 1$ , then it is consistent with order of accuracy  $p \geq 1$  in space and  $q \geq 1$  in time.

(ii) The sum of its first characteristic polynomial equals zero. That is

$$\sum_{j=0} \alpha_j = 0,$$

All the numerical schemes discussed above are found to have satisfied these conditions, hence the schemes are consistent.

### 2.2.3 Matrix Notation

In this chapter, our interest is beyond the use of finite difference formula to solve a system of PDEs. Since differentiation and finite difference approximation are linear operations, another way of representing the approximation to the differential operator is with the use of a matrix called differentiation matrix, see Trefethen [43, 44]. For example, using second-order centred finite difference approximation for the spatial discretization on the uniform grid of  $N + 1$  points, reduces the problem to  $N - 1$  coupled system of ordinary differential equations. Thus, the differentiation matrix with any given non-periodic boundary condition for the second derivative, form a **tridiagonal** matrix of the form

$$\mathbf{L} = \frac{1}{\Delta x^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & & \\ 0 & 0 & 0 & 0 & \dots & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 1 & -2 \end{pmatrix}_{(N-1) \times (N-1)} \quad (2.2.21)$$

In the same way, for the fourth-order centred finite difference approximation, the differentiation matrix representing the second derivative is **pentadiagonal** matrix of the form

$$\mathbf{L} = \frac{1}{12\Delta x^2} \begin{pmatrix} -30 & 16 & -1 & \dots & 0 & 0 & 0 \\ 16 & -30 & 16 & \dots & 0 & 0 & 0 \\ -1 & 16 & -30 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -30 & 16 & -1 \\ 0 & 0 & 0 & \dots & 16 & -30 & 16 \\ 0 & 0 & 0 & \dots & -1 & 16 & -30 \end{pmatrix}_{(N-1) \times (N-1)} \quad (2.2.22)$$

In a similar fashion, we can represent higher order finite difference approximations for the second, third and other higher derivatives in PDE problem. For the periodic boundary conditions,  $\mathbf{L}$  is of the same form but has a 1 in both top right and bottom left corners. Matrix  $\mathbf{L}$  form what is called **Toeplitz** matrix in which the order of the approximation determines the sparsity of the matrix.

**Definition 2.2.3** A Toeplitz matrix is a matrix in which each ascending diagonal from left to right has constant entries, that is, a matrix of the form

$$\mathbf{L} = \begin{pmatrix} l_0 & l_1 & l_2 & \dots & l_{N-1} \\ l_{-1} & l_0 & l_1 & \ddots & \vdots \\ l_{-2} & l_{-1} & l_0 & \ddots & l_2 \\ \vdots & \ddots & \ddots & \ddots & l_1 \\ l_{N+1} & \dots & l_{-2} & l_{-1} & l_0 \end{pmatrix}, \quad (2.2.23)$$

where the entries of  $\mathbf{L}$  satisfy the following property:

$$l_{ij} = l_{j-i}, \quad (2.2.24)$$

then  $\mathbf{L}$  is said to be a circulant matrix with eigenvalues given by

$$\lambda = \sum_{j=1}^N l_j e^{i2\pi(j-1)\frac{n}{N}}, \quad \text{for } n = 0, 1, \dots, N-1. \quad (2.2.25)$$

**Definition 2.2.4** Consider the following sequence:

$$s = \{l_k : k = -p, \dots, -1, 0, 1, \dots, q\}, \quad (2.2.26)$$

where  $p$  and  $q$  are positive integers. A square Toeplitz matrix  $\mathbf{L}$  of order  $N$  is of bandwidth  $(p + q + 1) \leq N$  if its entry  $l_{ij}$  is a member of the sequence  $s$  and zero otherwise. For instance, if  $p = q = 2$ ,  $\mathbf{L}$  is a pentadiagonal Toeplitz matrix.

We are primarily concerned in the eigenvalues of Toeplitz matrices obtained from the finite difference schemes. It will also be of paramount importance for determining the linear stability of our problems. The eigenvalues of a tridiagonal Toeplitz matrix of arbitrary order  $N$  are well understood, Mitchell [33]. The major challenge rest upon the Toeplitz matrix with higher bandwidth, the eigenvalue problems become intractable, see, for instance, the work of Sogabe [36, 37], although some algorithms have been derived for pentadiagonal matrices, see Cinkir [2], Kilic and El-Milkkawy [18] and El-Milkkawy [6] for details. An attempt to circumvent the difficulty in finding the eigenvalues of higher bandwidth Toeplitz matrices, we shall concentrate basically on the eigenvalues of the circulant Toeplitz matrices, which is more importantly related to our assumption of periodic boundary conditions.

## 2.3 Numerical Stability and Convergence Analysis

The stability of numerical schemes is closely associated with numerical error. A finite difference scheme is stable if the errors made at one time step of the calculation do not cause the errors to increase as the computations are continued. A neutrally stable scheme is one in which errors remain constant as the computations are carried forward. If the errors decay and eventually damp out, the numerical scheme is said to be stable. If, on the contrary, the errors grow with time the numerical scheme is said to be unstable.

The analytical solution  $u(x_m, t_n)$  of the differential equation, the difference solution  $u_m^n$  of the difference equation and the numerical solution  $\bar{u}_m^n$  can be related by the relation of the form

$$|u(x_m, t_n) - \bar{u}_m^n| \leq |u(x_m, t_n) - u_m^n| + |u_m^n - \bar{u}_m^n|. \quad (2.3.1)$$

In a computation, it is reasonable to expect the difference between the analytical and the numerical solution to be small. It is clear from (2.3.1) that this difference depends on the values  $|u(x_m, t_n) - u_m^n|$  and  $|u_m^n - \bar{u}_m^n|$ . We refer to the value  $|u(x_m, t_n) - u_m^n|$  as the local truncation error that arises as a result of the replacement of the differential equation with the difference equation. For a convergent difference scheme, the truncation error converges to zero as  $h$  and  $k$  both approach zero. The numerical error  $|u_m^n - \bar{u}_m^n|$  arises because in actual computation, we cannot solve the difference equation exactly because of the round-off errors. By stability, we mean the errors made at one stage of calculations do not cause increasingly large errors as the computations are progressed, but rather will eventually damp out. If the difference scheme is stable, then the second term in (2.3.1) is practically going to zero. Thus, the results of the convergent and stable methods are very close to the analytical values. We shall now discuss the stability and convergence of some of the schemes considered in this work.

There are two ways of examining the stability of a finite difference scheme. In one, the use of Fourier method and the second method, where the difference equations are expressed in matrix form and examine the eigenvalues of the associated matrix. The Fourier series method is much more appropriate for our own case in this work because of the nature of the boundary conditions of the problems we are considering.

### 2.3.1 Von Neumann (Fourier Series) Stability Analysis

For time-dependent problems, stability guarantees that the numerical method produces a bounded solution whenever the solution of the exact differential equation is bounded. Stability, in general, can be difficult to investigate, especially when the equation under consideration is nonlinear.

One useful and simple method of finding a stability criterion for a finite difference scheme is to construct a Fourier analysis of the difference equation and thereby derive the amplification factor. This technique is known as von Neumann's method.

In certain cases, von Neumann stability is necessary and sufficient for stability in the sense of Lax–Richtmyer (as used in the Lax equivalence theorem). The PDE and the finite difference scheme models are linear; the PDE is constant-coefficient with periodic boundary conditions and have only two independent variables; and the scheme uses no more than two time levels. Von Neumann stability is necessary in a much wider variety of cases. It is often used in place of a more detailed stability analysis to provide a good guess at the restrictions (if any) on the step sizes used in the scheme because of its relative simplicity.

**Second-order finite difference method:** We begin with von Neumann stability analysis that is based on the decomposition of errors into a Fourier series by considering first the second-order symmetric scheme. Let us consider the parabolic partial differential equation with one spatial independent variable

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + ru(1 - \frac{u}{\kappa}) \quad (2.3.2)$$

known as the Fisher equation. By using forward difference in time with central difference in space (FTCS), the discretized form of (2.3.2) on a spatial interval is written as

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \alpha \frac{(u_{j+1}^n - 2u_j^n + u_{j-1}^n)}{\Delta x^2} + u_j^n(1 - u_j^n), \quad (2.3.3)$$

by assuming that both  $r, \kappa = 1$ , which on further simplification leads to

$$u_j^{n+1} = u_j^n \omega (u_{j+1}^n - 2u_j^n + u_{j-1}^n) + \Delta t u_j^n (1 - u_j^n), \quad (2.3.4)$$

where  $\omega = \alpha \frac{\Delta t}{\Delta x^2}$ . We define the round-off error  $\xi_j^n$  as

$$\xi_j^n = U_j^n - u_j^n \quad (2.3.5)$$

we use  $u_j^n$  to denote the solution of the discretized equation (2.3.4) that is expected to be computed in the absence of round-off error, and  $U_j^n$  is the numerical solution obtained in finite precision arithmetic. The exact solution  $u_j^n$  is expected to satisfy the discretized equation exactly, so also for the error equation. Thus, we express the corresponding recurrence relation for the error in (2.3.4) as

$$\xi_j^n = \xi_j^n \omega (\xi_{j+1}^n - 2\xi_j^n + \xi_{j-1}^n) + \Delta t \xi_j^n (1 - \xi_j^n). \quad (2.3.6)$$

Equations (2.3.4) and (2.3.6) indicate that the error and the numerical solution have the same growth or decay behaviour with respect to time. For linear differential

equations with periodic boundary condition, the spatial variation of error may be expanded in a finite Fourier series in the interval  $l$  as

$$\xi(x) = \sum_{m=1}^M A_m e^{ik_m x}, \quad (2.3.7)$$

where  $k_m = \pi/l$  is the wavenumber with  $m = 1, 2, \dots, M-1, M$  and  $M = l/\Delta x$ . The time dependence of the error is included by assuming that the amplitude of error  $A_m$  is a function of time. It is reasonable to assume that the amplitude varies exponentially with time, since the error tends to grow or decay exponentially with time, hence we can express (2.3.7) in the form

$$\xi(x, t) = \sum_{m=1}^M e^{at} e^{ik_m x} \quad (2.3.8)$$

with  $a$ , a constant. We can consider the growth of error of a particular term since the difference equation for error is linear, we expect the behaviour of each term of the series in (2.3.8) to be the same as series itself, so

$$\xi(x, t) = e^{at} e^{ik_m x}. \quad (2.3.9)$$

Without loss of generality, the stability characteristic can be studied in this form. On substituting (2.3.9) into (2.3.8) into (2.3.4), noting how individual terms

$$\begin{aligned} \xi_j^n &= e^{at} e^{ik_m x} \\ \xi_j^{n+1} &= e^{a(t+\Delta t)} e^{ik_m x} \\ \xi_{j+1}^n &= e^{at} e^{ik_m(x+\Delta x)} \\ \xi_{j+1}^n &= e^{at} e^{ik_m(x-\Delta x)} \end{aligned}$$

after further simplification, Eq. (2.3.6) reduces to

$$e^{a\Delta t} = 1 + \omega(e^{ik_m \Delta x} + e^{-ik_m \Delta x} - 2). \quad (2.3.10)$$

By using the identities, we can express the term  $e^{ik_m \Delta x}$  in terms of  $\cos(k_m \Delta x) + i \sin(k_m \Delta x)$ , so that

$$\cos(k_m \Delta x) = \frac{e^{ik_m \Delta x} + e^{-ik_m \Delta x}}{2}, \quad \sin^2\left(\frac{k_m \Delta x}{2}\right) = \frac{1 - \cos(k_m \Delta x)}{2},$$

then (2.3.10) becomes

$$e^{a\Delta t} = 1 - 4\omega \sin^2\left(\frac{k_m \Delta x}{2}\right). \quad (2.3.11)$$

We define the amplification factor

$$G \equiv \frac{\xi_j^{n+1}}{\xi_j^n}.$$

The necessary and sufficient condition for the error to remain bounded is that

$$G \leq 1.$$

However,

$$G = \frac{e^{\alpha(t+\Delta t)} e^{ik_m x}}{e^{\alpha t} e^{ik_m x}} = e^{\alpha \Delta t}. \quad (2.3.12)$$

From Eqs. (2.3.11) and (2.3.12), we give the stability condition as

$$\left| 1 - 4\omega \sin^2 \left( \frac{k_m \Delta x}{2} \right) \right| \leq 1, \quad (2.3.13)$$

since this condition must hold for every wavenumber  $k_m$ , we take a minimum value of the sine functions so that  $1 - 4\omega \geq -1$  and  $\omega \geq 0$ , of course, for  $\omega = 0$ , it implies that  $\Delta t = 0$ , which is impractical. Thus, we have  $0 < \omega \leq 1/2$  where  $\omega$  remains as earlier defines. In order to ensure a stable solution or reduce errors, maximum care must be exercised in selecting the value of  $\omega$ . It further implies that for a given  $\Delta x$ , the allowed value of  $\Delta t$  must be small enough to satisfy  $\omega \leq 1/2$ . We conclude by saying that a finite difference equation is stable if it produces a bounded solution when the exact solution is bounded, and is unstable if it produces an unbounded solution when the exact solution is bounded.

**Fourth-order finite difference method:** Just as we have done for the second-order method above, we shall repeat the same process for the fourth-order method, given consideration to diffusion equation (2.3.2). We use fourth-order central difference for the first derivative in time and another fourth-order central difference for the second derivative in space, we refer to this method as CTCS(4,4). We have Eq. (2.3.2) written in the form

$$-u_j^{n+2} + 8u_j^{n+1} - 8u_j^{n-1} + u_j^{n-2} = \omega(-u_{j+2}^n + 16u_{j+1}^n - 30u_j^n + 16u_{j-1}^n - u_{j-2}^n) + \Delta t u_j^n (1 - u_j^n), \quad (2.3.14)$$

where

$$\omega = \alpha \frac{\Delta t}{\Delta x^2} \quad (2.3.15)$$

is called the *Courant number*.

In order to determine the Courant–Friedrichs–Levy (CLF) condition for the stability of (2.3.14) via von Neumann stability analysis, to achieve this we assume that  $u_j^n = \xi^n e^{ikjh}$  where  $\xi$  represents the time dependence of the solution and the exponential represents the spatial dependence. Exponential  $jh$  represents the position

along the grid and  $k$  is the spatial wave number in this case. It is assumed that the coefficients in the equation are varying slowly that they may be considered in both space and time. So, on substituting this we have the corresponding error equation expressed as

$$-\xi_j^{n+2} + 8\xi_j^{n+1} - 8\xi_j^{n-1} + \xi_j^{n-2} = \omega(-\xi_{j+2}^n + 16\xi_{j+1}^n - 30\xi_j^n + 16\xi_{j-1}^n - \xi_{j-2}^n) + \xi_j^n(1 - \xi_j^n), \quad (2.3.16)$$

we let

$$\xi(j, n) = \xi^n e^{ikjh} \quad (2.3.17)$$

On substituting (2.3.17) into (2.3.16) gives

$$\begin{aligned} & -\xi^{n+2} e^{ikjh} + 8\xi^{n+1} e^{ikjh} - 8\xi^{n-2} e^{ikjh} + \xi^{n-2} e^{ikjh} \\ & = \omega \left[ -\xi^n e^{ik(j+2)h} + 16\xi^n e^{ik(j+1)h} - 30\xi^n e^{ikjh} \right. \\ & \quad \left. + 16\xi^n e^{ik(j-1)h} - \xi^n e^{ik(j-2)h} + \xi^n e^{ikjh} (1 - \xi^n e^{ikjh}) \right]. \end{aligned} \quad (2.3.18)$$

Dividing by  $\xi^n e^{ik(j-2)h}$  and further simplification reduces (2.3.18) to

$$-\xi^4 + 8\xi^3 - 8\xi + 1 = \omega \left[ -e^{2ikh} + 16e^{ikh} - 30 + 16e^{-ikh} - e^{-2ikh} \right] \xi^2, \quad (2.3.19)$$

or

$$\xi^4 - 8\xi^3 - \omega \left[ -e^{2ikh} + 16e^{ikh} - 30 + 16e^{-ikh} - e^{-2ikh} \right] \xi^2 + 8\xi - 1 = 0, \quad (2.3.20)$$

we set

$$e^{ikh} = e^{i\theta} = \cos \theta + i \sin \theta,$$

with this identity our last equation is reduced to

$$\xi^4 - 8\xi^3 - \omega(-2 \cos 2\theta + 32 \cos \theta - 30)\xi^2 + 8\xi - 1 = 0. \quad (2.3.21)$$

In a more compact form, we have the amplification polynomial

$$\xi^4 - 8\xi^3 - \omega G \xi^2 + 8\xi - 1 = 0, \quad (2.3.22)$$

where  $G = -2 \cos 2\theta + 32 \cos \theta - 30$ . We can see at this point that as the degree of polynomial is increased, so also the complexity of solving the problem itself. With the aid of a MATHEMATICA program, we resolve (2.3.22) as

$$\begin{aligned}
\xi_1 &= -2 - \frac{\sqrt{14 + \psi}}{2} - \frac{1}{2} \sqrt{34 + \psi - \frac{-448 - 32\psi}{4\sqrt{14 + \psi}}} \\
\xi_2 &= -2 - \frac{\sqrt{14 + \psi}}{2} + \frac{1}{2} \sqrt{34 + \psi - \frac{-448 - 32\psi}{4\sqrt{14 + \psi}}} \\
\xi_3 &= -2 + \frac{\sqrt{14 + \psi}}{2} - \frac{1}{2} \sqrt{34 + \psi - \frac{112}{\sqrt{14 + \psi}} - \frac{8\psi}{\sqrt{14 + \psi}}} \\
\xi_4 &= -2 + \frac{\sqrt{14 + \psi}}{2} + \frac{1}{2} \sqrt{34 + \psi - \frac{112}{\sqrt{14 + \psi}} - \frac{8\psi}{\sqrt{14 + \psi}}}, \quad (2.3.23)
\end{aligned}$$

with  $\psi = \omega G$ . Ordinarily, for solution to be stable in time we must have  $|\xi_i| \leq 1$ , for  $i = 1(1)4$ . Otherwise, since  $n$  is a positive integer,  $\xi^n$  will be a rapid growing value. So we look for the largest possible value of  $|\xi|$  and find the condition to keep it  $\leq 1$ . By intermediate value theorem, we let

$$g(\xi) = \xi^4 - 8\xi^3 - \omega G \xi^2 + 8\xi - 1,$$

which is a continuous function. We want to show that there exists a root  $\xi \leq 1$  for  $g(x) = 0$  on  $[0, 1]$ . We now observe that

$$g(0) = -1 < 0 \quad \text{and} \quad g(1) = -\omega G$$

with possibility of cases (i)  $\omega G > 0$ , (ii)  $\omega G = 0$ , and (iii)  $\omega G < 0$ . It is obvious that the scheme presented here will only satisfy the stability condition if the value  $|\xi G| \leq 1$ , so the scheme is conditionally stable.

Again, we verify further by using backward difference approximation in time coupled with central difference in space BTCS(1,4) for the first and second derivatives, respectively, in Eq. (2.3.2). Thus,

$$u_j^n - u_j^{n-1} = \omega[-u_{j+2}^n + 16u_{j+1}^n - 30u_j^n + 16u_{j-1}^n - u_{j-2}^n] + u_j^n(1 - u_j^n), \quad (2.3.24)$$

where  $\omega = D\Delta t/12\Delta x^2$ . By assuming

$$u_j^n = g^n e^{ikh},$$

then after some algebraic simplification, Eq. (2.3.24) reduces to

$$g - 1 = \omega[-u^{2ikh} + 16u^{ikh} - 30 + 16u^{-ikh} - u^{-2ikh}]g, \quad (2.3.25)$$

we factorize for  $g$  and set  $e^{ikh} = e^{i\theta}$  so that (2.3.24) becomes

$$g(1 - \omega(-2\cos 2\theta + 32\cos \theta - 30)) = 1, \quad (2.3.26)$$

or

$$g = \frac{1}{1 - \omega(-2 \cos 2\theta + 32 \cos \theta - 30)}. \quad (2.3.27)$$

Clearly,  $g \leq 1$ . This method describes here which is first order in time and fourth order in space, is unconditionally stable for any value of  $\omega$  in the entire computational domain.

The choices  $s = 0$ ,  $d = 2$ ,  $n = 2$  and  $m = 2$ , produce the output

$$\left\{ \left\{ \frac{h^2}{12}, \frac{5h^2}{12}, \frac{h^2}{12} \right\}, \{1, -2, 1\} \right\}$$

corresponding to the implicit fourth-order accurate formula for the second derivative

$$\frac{u(x+1) - 2u(x) + u(x-1)}{h^2} \approx \frac{1}{12}u''(x+1) + \frac{5}{6}u''(x) + \frac{1}{12}u''(x-1). \quad (2.3.28)$$

On applying (2.3.28) to discretize (2.3.2), we have

$$u_j^{n+1} - 2u_j^n + u_j^{n-1} = \omega[u_{j+1}^n + 10u_j^n + u_{j-1}^n] + u_j^n(1 - u_j^n), \quad (2.3.29)$$

where  $\omega = h^2/12$ . To analyse the stability of (2.3.29), we assume as usual that  $u_j^n = g^n e^{ij\theta}$  and therefore substitute accordingly to have

$$\begin{aligned} g^{n+1} e^{ij\theta} - 2g^n e^{ij\theta} + g^{n-1} e^{ij\theta} &= \omega[g^n e^{i(j+1)\theta} + 10g^n e^{ij\theta} + g^n e^{i(j-1)\theta}] \\ &\quad + g^n e^{ij\theta}(1 - g^n e^{ij\theta}), \end{aligned} \quad (2.3.30)$$

which on further simplifications, reduces to

$$g^2 - (\omega[2 \cos \theta + 10]g - 2)g + 1 = 0 \quad (2.3.31)$$

as the amplification equation with roots

$$\begin{aligned} g &= \frac{1}{2} \left( 2 - 10\omega - 2\omega \cos \theta - \sqrt{-4 + (-2 + \omega(10 + 2 \cos \theta))^2} \right) \\ \text{or} \\ g &= \frac{1}{2} \left( 2 - 10\omega - 2\omega \cos \theta + \sqrt{-4 + (-2 + \omega(10 + 2 \cos \theta))^2} \right). \end{aligned} \quad (2.3.32)$$

In both cases, it is clear that irrespective of what value is assigned to  $\omega$ ,  $g \leq 1$ . Hence, the method is stable.

The CFL condition introduced by Courant et al. [3] implies that the scheme is unstable when  $\alpha \Delta t \leq \Delta x$ , which agrees with our findings in each of the cases considered. Explicit schemes have the desirable property that solutions can be computed cheaply as one moves from each time level to the next. Nevertheless, for any explicit

scheme, the CFL condition places a restriction on the maximum permissible time step. Thus if the mesh in the  $x$ -direction is fine (a situation that might arise at a boundary layer), then large time steps will not be permitted, and consequently, an excess of computational effort may be needed to reach  $initial\ time(t) = final\ time(T)$ .

More work per time step is needed when one uses an implicit scheme. This may be offset by the fact that implicit schemes generally have much less restrictive conditions (or perhaps none at all) on the maximum permissible value of  $\Delta t$ . *The CFL condition requires that the numerical domain of dependence of a finite-difference scheme include the domain of dependence of the associated partial differential equation.* Satisfaction of the CFL condition is a necessary condition for stability, but is not sufficient to guarantee stability.

### 2.3.2 Matrix Stability Analysis

Before going to discussion of matrix stability analysis per se, it is important to talk briefly about matrices and vectors that are used in this work as many of the applications of linear algebra in the text, for instance, Leveque [23], Strikwerda [40] Trefethen [43], Trefethen and Embere [45] used vectors with complex components. We denote the set of complex numbers by  $\mathbb{C}$ .

Let us consider a vector,  $u$ , as contained in our situation, as an element of  $\mathbb{C}^M$ , that is,  $u = (u_1, u_2, \dots, u_M)$ , where  $u_j$ , the  $j$ th component of  $u$ , is a complex number. Norms are defined as real-valued functions on a vector space that provide a notation of the length of a vector. For example, the most common norms often considered are the Euclidean norm denoted by  $\ell^2$  and defined as

$$|u|_2 = \sqrt{\left(\sum_{j=1}^M |u_j|^2\right)},$$

the  $\ell^1$  norm,

$$|u|_1 = \left(\sum_{j=1}^M |u_j|\right),$$

and the third class which is the  $\ell^\infty$ , called maximum norm,

$$|u|_\infty = \max_{1 \leq j \leq M} |u_j|.$$

Three important properties that are satisfied by each of these norms are; (i)  $|u| \geq 0$ , with equality if and only if  $u = 0$ . (ii)  $|u + \omega| \leq |u| + |\omega|$ , and (iii)  $|\alpha u| = |\alpha||u|$  for  $\alpha \in \mathbb{C}$ . The proof of these properties are exempted in this work, readers are

referred to Bahouri [1], Holden and Karlsen [15], Hoffman [14] and Thomas [41, 42], and the references therein.

An  $M \times N$  matrix is defined as a linear map from  $\mathbb{C}^M$  to  $\mathbb{C}^N$ . We can write the  $(i,j)$ th component of a matrix, say  $A$  in the form  $A_{ij}$  or simply  $a_{ij}$ , where  $a_{ij}$  is defined as the  $i$ th component of  $Ae_j$ . By definition, the transpose of an  $M \times N$  matrix  $A$  is the  $N \times M$  matrix  $A^T$ , given as

$$(A^T)_{ij} = \bar{A}_{ji},$$

where  $T$  and bar stand for the transpose and complex conjugate, respectively.

On considering both  $\mathbb{C}^M$  and  $\mathbb{C}^N$  with norms, we can define the norm of an  $M \times N$  of matrix  $A$  by

$$\|A\| = \sup_{|u|=1} |Au| = \sup_{u \neq 0} \frac{|Au|}{|u|}, \quad (2.3.33)$$

where  $|Au|$  and  $|u|$  are the respective norms of  $\mathbb{C}^M$  and  $\mathbb{C}^N$ . Equivalence expressions in (2.3.33) follow from the linearity of  $A$  and property (iii) mentioned earlier. In this manner, the norm defined on the vector space  $M \times N$  matrices is satisfied.

Another important aspect of a our matrix we need to mention is its nature, whether it is positive definite, hermitian or symmetric. Matrix  $A$  is positive and semi-definite for  $A \geq 0$  if  $\langle u, Au \rangle \geq 0$  for all vectors  $u$ . We can deduce that  $A \geq B$  if  $A - B \geq 0$ . For instance, if  $A \geq 0$ , then  $\alpha A \geq 0$  for all positive number  $\alpha$ , and  $A \geq 0$  and  $B \geq 0$ , this implies that their sum, that is,  $A + B \geq 0$ . So also, if  $A \leq B$ , then  $B \geq A$ . A matrix is said to be negative definite or negative semi-definite if  $-A$  is, respectively, positive definite or positive semi-definite. Our proposed fourth-order central finite difference leads to a symmetric matrix. By definition, if all the components of a hermitian matrix are real numbers, then the matrix is called a symmetric matrix. There is an extensive literature on iterative methods for solving a linear system

$$Ax = b \quad (2.3.34)$$

which requires to decompose the matrix  $A$  by writing it as

$$A = B - C \quad (2.3.35)$$

and then solve the system of equations

$$Bx^{k+1} = Cx^k + b \quad (2.3.36)$$

iteratively. In the present case, the matrix  $A$  representing the scheme is symmetric when the coefficient multiplying  $\nu_{n',m'}$  in the scheme applied at grid point  $(n, m)$  is the same as the coefficient multiplying  $\nu_{n,m}$  in the scheme applied at grid point

$(n', m')$  for each of the unknown grid function values. The main result for symmetric, positive definite matrices is buttressed by the following theorem.

**Theorem** *If  $A$  is symmetric and positive definite, then the iterative method (2.3.36) based on the splitting (2.3.35) is convergent if*

$$ReB > \frac{1}{2}A \quad (2.3.37)$$

or, equivalently, that  $B^T + C > 0$  is symmetric and positive definite, that is,

$$B^T + C > 0. \quad (2.3.38)$$

*Proof* We follow closely the proof as established in [40], where the matrix  $ReB$  is assumed to be  $(B + B^T)/2$  in such a way that (2.3.37) is equivalent to

$$B^T + B - A > 0. \quad (2.3.39)$$

□

The relation defined in (2.3.35) gives an indication that it is equivalent to (2.3.38) and that  $B^T + C$  is also symmetric. To begin with, the error in the norm is measured by  $A$ , this means that  $\|x\|_A = \sqrt{(x, Ax)}$ . With this norm, we have a relation

$$\|err^{k+1}\|_A = \|B^{-1}Cerr^k\|_A \leq \|B^{-1}C\|_A \|err^k\|_A.$$

It follows that if the norm  $B^{-1}C$  is less than one, then the error will decrease at each step of iteration and the method will converge. Hence, the norm  $B^{-1}C$  is defined by

$$\|B^{-1}C\|_A^2 = \sup_{x \neq 0} \frac{(B^{-1}Cx, AB^{-1}Cx)}{(x, Ax)} = \sup_{x \neq 0} \frac{(x, C^T B^{-T} AB^{-1}Cx)}{(x, Ax)}.$$

Obviously, the condition  $\|B^{-1}C\|_A < 1$  is equivalent to  $C^T B^{-T} AB^{-1}C < A$ , and by considering  $C^T B^T AB^{-1}C$ , using the relation in (2.3.35), we have

$$\begin{aligned} C^T B^{-T} AB^{-1}C &= (I - AB^{-T})A(I - B^{-1}A) \\ &= A - (AB^{-T}A + AB^{-1}A - AB^{-T}AB^{-1}A). \end{aligned}$$

Thus, we see that  $C^T B^{-T} AB^{-1}C < A$  if and only if

$$AB^{-T}A + AB^{-1}A - AB^{-T}AB^{-1}A > 0, \quad (2.3.40)$$

which when factorized gives  $AB^{-T}(B + B^T - A)B^{-1}A$ . Clearly, we can assert that (2.3.40) is true if and only if (2.3.39) is satisfied. This implies that  $\|B^{-1}\|_A$  is less than one, therefore the method is convergent.

Using the given boundary conditions, we consider a standard diffusion equation  $u_t = \sigma u_{xx}$ , its two level difference method is written as

$$A_0 u^{n+1} = A_1 u^n + b^n, \quad n = 0, 1, 2, \dots, \quad (2.3.41)$$

where  $b^n$  is expected to have contained the boundary conditions and  $|A_0| \neq 0$ . For  $A_0 = \mathbf{I}$ , the difference scheme (2.3.41) will be an explicit scheme, otherwise it is an implicit scheme. The components of  $u^0$  are the initial values from which the computation is started. We let  $\bar{u}^0$  be the amount of error introduced into  $u^0$ , so that the resulting equation now becomes

$$\begin{aligned} A_0 \bar{u}^1 &= A_1 \bar{u}^0 + b^0 \\ A_0 \bar{u}^2 &= A_1 \bar{u}^1 + b^1 \\ A_0 \bar{u}^3 &= A_1 \bar{u}^0 + b^2 \\ &\vdots \\ A_0 \bar{u}^n &= A_1 \bar{u}^{n-1} + b^{n-1} \\ A_0 \bar{u}^{n+1} &= A_1 \bar{u}^n + b^n, \quad n \geq 0. \end{aligned} \quad (2.3.42)$$

On subtracting (2.3.41) from the last equation in (2.3.42), we have

$$A_0 E r^{n+1} = A_1 E r^n, \quad n = 0, 1, 2, \dots, \quad (2.3.43)$$

where  $\bar{u}^n - u^n = E r^n$  is defined as the round-off error. In the stability analysis of the matrix method, we determine the conditions under which the error norm

$$\|E r^n\| = \|\bar{u}^n - u^n\|,$$

where  $\|\cdot\|$  indicates a stable norm, is bounded as  $n \rightarrow \infty$ , with  $k$  fixed.

Again, we can rewrite Eq. (2.3.43) in the form

$$E r^{n+1} = \xi E r^n, \quad n = 0, 1, 2, \dots, \quad (2.3.44)$$

where  $\xi = A_0^{-1} A_1$  and  $\xi$  is also called the amplification matrix. Setting  $n = 1, 2, 3, \dots$ , we have

$$\|E r^n\|^{n+1} \leq \|\xi\|^{n+1} \|E r^0\|. \quad (2.3.45)$$

Therefore, for the stability we require that

$$\|\xi\| \leq 1. \quad (2.3.46)$$

In this segment, the particular case is when  $\xi$  is symmetric matrix then  $\|\xi\|_2 = \rho(\xi)$  in such a way that Eq. (2.3.46) has an equivalence form

$$\rho(\xi) \leq 1, \quad (2.3.47)$$

where Hilbert norm is used. The condition in (2.3.47) satisfies von Neumann necessary condition for stability.

### 2.3.3 Convergence

A difference scheme is said to be convergent if

$$\lim_{k \rightarrow 0, nk \rightarrow t} u^n(x) = u(x, t) \quad (2.3.48)$$

for all  $x$  and  $t$  in the region of interest. It is assumed that  $u_j^n$  is free from the round-off errors, so that the only difference between  $u(x_j, tn)$  and  $u_j^n$  is the error made by replacing the differential equation by the difference equation, that is, we are talking about the local truncation error.

We begin the study of convergence by considering the diffusion equation

$$u_t = \sigma u_{xx}, \quad a \leq x \leq b, t > 0 \quad (2.3.49)$$

$$u(0, t) = g_1(t) \quad u(1, t) = g_M(t) \quad (2.3.50)$$

$$u(x, t = 0) = u_0(x), \quad (2.3.51)$$

where  $\sigma$  is the diffusion coefficient. Equation (2.3.49) can be written in a more compact form as

$$u_t = Lu, \quad (2.3.52)$$

where  $L$  is the differential operator in space direction. On applying forward formula of order  $O(h)$  in time and centred formula of order  $O(h^2)$  in space (FTCS), Eq. (2.3.49) becomes

$$u_j^{n+1} = \lambda u_{j-1}^n + (1 - 2\lambda)u_j^n + \lambda u_{j+1}^n + O(\Delta t + \Delta x^2), \quad j = 1, 2, \dots, M, \quad (2.3.53)$$

where  $\lambda = \sigma \Delta t / \Delta x^2$ . In our computation, we can simply write the linear system that results from Eq. (2.3.53) as

$$u^{n+1} = L_{\Delta}^A u^n. \quad (2.3.54)$$

If we use the backward difference at time  $t_{n+1}$  and a second-order central difference for the space derivative at position  $x_j$ . We denote their combination as the backward

time, centred space method (BTCS), when used to approximate (2.3.49) we get the recurrence equation

$$-\lambda u_{j-1}^{n+1} + (1 - 2\lambda)u_j^{n+1} - \lambda u_{j+1}^{n+1} = u_j^n + O(\Delta t + \Delta x^2), \quad j = 1, 2, \dots, M. \quad (2.3.55)$$

The linear system that results from (2.3.55) can be presented as

$$u^{n+1} = (L_{\Delta}^B)^{-1}u^n. \quad (2.3.56)$$

The third class is obtained by using the central difference at time  $t_{n+1/2}$  and a second-order central difference for the space derivative at position  $x_j$  (CTCS), we get the recurrence equation of the form

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{1}{2} \left( \frac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{\Delta x^2} + \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} \right). \quad (2.3.57)$$

This formula is well referred to as the popular Crank–Nicholson scheme. By applying (2.3.57) to approximate (2.3.49), we have

$$-\frac{\lambda}{2}u_{j-1}^{n+1} + (1 + \lambda)u_j^{n+1} - \frac{\lambda}{2}u_{j+1}^{n+1} = \frac{\lambda}{2}u_{j-1}^n + (1 - \lambda)u_j^n + \frac{\lambda}{2}u_{j+1}^n \quad (2.3.58)$$

with local truncation error of order  $O(\Delta t^2 + \Delta x^2)$ . Compactly, we may also write the linear system of (2.3.58) as

$$u^{n+1} = (L_{\Delta}^C)^{-1}L_{\Delta}^D u^n = (L_{\Delta}^{EN})u^n. \quad (2.3.59)$$

By replacing  $\Delta t \rightarrow k$  and  $\Delta x \rightarrow h$ , and expanding each term in (2.3.53) in Taylor's series, we find the truncation error ( $E_{trunc}$ ) of the formula as

$$\begin{aligned} E_{trunc} &= u(x_j, t_{n+1}) - u(x_j, t_n) - \lambda[u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n)] \\ &= \left[ \left( k\delta_t + \frac{k^2}{2}\delta_{tt} + \dots \right) - \frac{k}{h^2} \left( h^2\delta_x^2 + \frac{h^4}{12}\delta_x^4 \right) \right] \\ &= \frac{k^2}{2}u_{tt} - \frac{kh^2}{12}\delta_x^4 u + O(k^3 + kh^4), \end{aligned} \quad (2.3.60)$$

where  $\delta t = \partial/\partial t$  and  $\delta x = \partial/\partial x$ . The  $E_{trunc}$  of the method is of order  $O(k^2 + kh^2)$ . The *order* of the method is given as

$$\frac{1}{k}(E_{trunc}) = O(k + h^2).$$

If the solution of the difference equation tends to the solution of the differential equation as  $h \rightarrow 0$  and  $k \rightarrow 0$ , then the difference equation is said to be *convergent*. For illustration, we can write the exact solution to difference approximation (2.3.53) in the form

$$u(x_j, t_{n+1}) = u(x_j, t_n) + \lambda \delta_x^2 u(x_j, t_n) + O(k^2 + kh^2), \quad (2.3.61)$$

on setting  $Er_n^j = u(x_j, t_n) - u_j^n$  and  $E^n = \max_j |Er_n^j|$ . On subtracting Eq. (2.3.53) from Eq. (2.3.53), we have

$$Er_j^{n+1} = (1 - 2\lambda)Er_j^n + \lambda(Er_{j-1}^n + Er_{j+1}^n) + G(k^2 + kh^2),$$

we expect that the constant  $G$  is independent of  $h$ . For  $\lambda < 1/2$ , the values of the coefficients are positive and

$$\max_j |Er_j^{n+1}| \leq (1 - 2\lambda + \lambda + \lambda) \max_j |Er_j^n| + G(k^2 + kh^2).$$

Thus, we have

$$\begin{aligned} E^{n+1} &\leq E^n + G(k^2 + kh^2) \\ &\leq E^{n-1} + 2G(k^2 + kh^2) \\ &\quad \vdots \quad \quad \quad \vdots \\ &\leq E^0 + (n+1)G(k^2 + kh^2) \\ &\leq t_{n+1}G(k^2 + kh^2). \end{aligned} \quad (2.3.62)$$

When  $t_{n+1} = (n+1)k$  and  $E^0 = 0$ , for  $h \rightarrow 0, k \rightarrow 0$ , we get

$$E^{n+1} \rightarrow 0$$

and that

$$u_j^n \rightarrow u(x_j, t_n).$$

Hence, we say that the method is convergent.

Again, on substituting  $Er_n^j = u_j^n - u(x_j, t_n)$  in (2.3.58), we get the error equation as

$$\left(\mathbf{I} + \frac{\lambda}{2}\mathbf{J}\right) Er^{n+1} = \left(\mathbf{I} - \frac{\lambda}{2}\mathbf{J}\right) Er^n + \mathbf{T}^n, \quad n = 0, 1, 2, \dots, \quad (2.3.63)$$

where the Jacobian  $\mathbf{J}$  is regarded as a community matrix and

$$\begin{aligned} Er^n &= [Er_1^n, Er_2^n, \dots, Er_{j-1}^n]^T \\ \mathbf{T}^n &= [T_1^n, T_2^n, \dots, T_{j-1}^n]^T \\ T_j^n &= O(k^3 + kh^2) \end{aligned}$$

$$\mathbf{J} = \begin{pmatrix} 2 & -1 & & & \mathbf{0} \\ -1 & -2 & -1 & & \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ & & & -1 & -2 & -1 \\ \mathbf{0} & & & & -1 & 2 \end{pmatrix}$$

we can write (2.3.63) compactly as

$$Er^{n+1} = \mathbf{A}Er^n + \zeta^n, \quad n = 0, 1, 2, \dots, \quad (2.3.64)$$

where

$$\mathbf{A} = \left( \mathbf{I} + \frac{\lambda}{2} \mathbf{J} \right)^{-1} \left( \mathbf{I} - \frac{\lambda}{2} \mathbf{J} \right)$$

and

$$\zeta^n = (\mathbf{I} + \lambda^2 \mathbf{J})^{-1} \mathbf{T}^n.$$

Recursive application of (2.3.64) yields

$$Er^{n+1} = \mathbf{A}^n Er^0 + \sum_{a=1}^n \mathbf{A}^{n-a} \zeta^{a-1}, \quad n = 0, 1, 2, \dots \quad (2.3.65)$$

This means in other words that

$$\begin{aligned} \|Er^n\| &\leq \|\mathbf{A}\|^n \|Er^0\| + \sum_{a=1}^n \|\mathbf{A}\|^{n-a} \|\zeta^{a-1}\| \\ &\leq \|\mathbf{A}\|^n \|Er^0\| + \frac{1 - \|\mathbf{A}\|^n}{1 - \|\mathbf{A}\|} \left( \max_{0 \leq m \leq n-1} \|\zeta^m\| \right). \end{aligned} \quad (2.3.66)$$

Since in all our cases, the matrix  $\mathbf{J}$  is symmetric, so also the matrix  $\mathbf{A}$  is symmetric. By virtue of the spectral norm, we have

$$\|\mathbf{A}\| = \max_j |\varphi_j|, \quad (2.3.67)$$

where  $\lambda_j$ ,  $1 \leq j \leq M-1$  are the eigenvalues of  $\mathbf{J}$ . The eigenvalues  $\lambda_j$  of symmetric matrix  $\mathbf{J}$  are given by

$$\lambda_j = 4 \sin^2(j\pi/2M), \quad 1 \leq j \leq M-1$$

also,  $\varphi_j$ ,  $1 \leq j \leq M - 1$  are the eigenvalues of  $\mathbf{A}$ . The eigenvalues of  $\mathbf{A}$  are given by

$$\varphi_j = \left(1 + \frac{\lambda}{2}\lambda_j\right)^{-1} \left(1 - \frac{\lambda}{2}\lambda_j\right). \quad (2.3.68)$$

Using Eqs. (2.3.67) and (2.3.68), we easily verified that

$$\mathbf{A} = \max_{1 \leq j \leq M-1} |\varphi_j| < 1, \quad \lambda > 0,$$

then Eq. (2.3.66) reduces to

$$\|Er^n\| \leq \|Er^0\| + \frac{1}{1 - \|\mathbf{A}\|} \left( \max_{0 \leq j \leq n-1} \|\mathbf{T}^j\| \right) \quad (2.3.69)$$

and

$$\max_{0 \leq j \leq n-1} \|\mathbf{T}^j\| = G(k^2 + h^2),$$

with  $G$  being a constant independent of  $k$  and  $h$ . Hence, we have

$$\|Er^n\| \leq \|Er^0\| + G(k^2 + h^2) \quad (2.3.70)$$

is unconditionally convergence as both  $k, h \rightarrow 0$ .

The above process can be repeated to examine the convergence of the fourth-order scheme, though the idea is tasking and more rigorous. Hence, we conclude with the definition of convergence Gedney [12] that says; *A finite difference equation (FDE) is consistent with a partial differential equation (PDE) if the difference between the FDE and the PDE (i.e. the truncation error) vanishes as the sizes of the time step  $k$  or  $\Delta t$  and spatial grid spacing  $h$  or  $\Delta x$  go to zero independently, is satisfied.* In addition, the Lax and Richtmyer [21] equivalence theorem states that ‘*a consistent finite-difference scheme for a partial differential equation for which the initial-value problem is well posed is convergent if and only if it is stable*’, for a proof, readers are referred to Strikwerda [40]. Finally, by Dahlquist equivalence theorem, ‘*a linear multistep formula is convergent if and only if it is consistent and stable*’.

### 2.3.4 Symmetry

According to Fatunla [7], Jain [16] and Lambert and Watson [20], method of the form (2.3.14) is said to be symmetric if when the values of  $\alpha'_j$ s and  $\beta'_j$ s are interchanged, the function is the same or is multiplied by minus one. Thus, method (2.3.14) is symmetric if

$$\alpha_j = \alpha_{J-j}, \quad \beta_j = \beta_{J-j}, \quad j = 0(1)J, \quad (2.3.71)$$

where  $\alpha_j$  and  $\beta_j$  correspond to the coefficients of the first and second characteristic polynomial of Eq. (2.3.14). It follows that

$$\begin{aligned}\alpha_0 &= -\alpha_4 = -1 \\ \alpha_1 &= -\alpha_3 = -8 \\ \alpha_2 &= -\alpha_2 = 0\end{aligned}$$

and

$$\begin{aligned}\beta_0 &= \beta_4 = -1 \\ \beta_1 &= \beta_3 = -16 \\ \beta_2 &= \beta_2 = 30\end{aligned}$$

Hence, the method is symmetric.

## 2.4 Numerical Results

Numerical method of solution discussed earlier is applied to solve both the diffusion equation (2.2.9) and the reaction–diffusion equation (2.3.2), subject to the initial condition

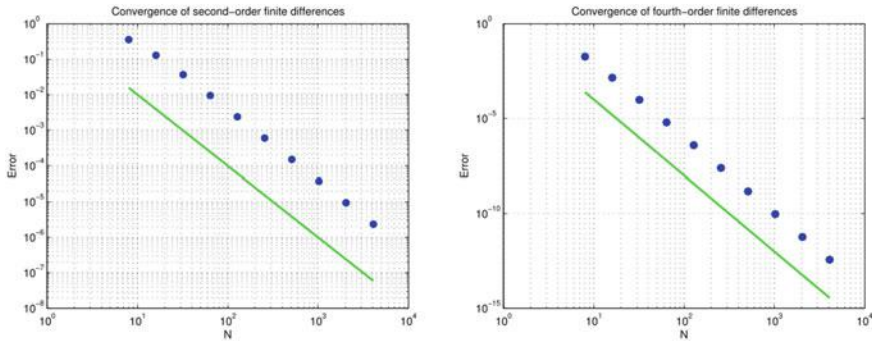
$$u(x, 0) = \frac{1}{\cosh(\delta x)}, \quad x \in [a, b] \quad (2.4.1)$$

and homogeneous Dirichlet boundary conditions

$$u(a, t) = u(b, t) = 0, \quad t > 0.$$

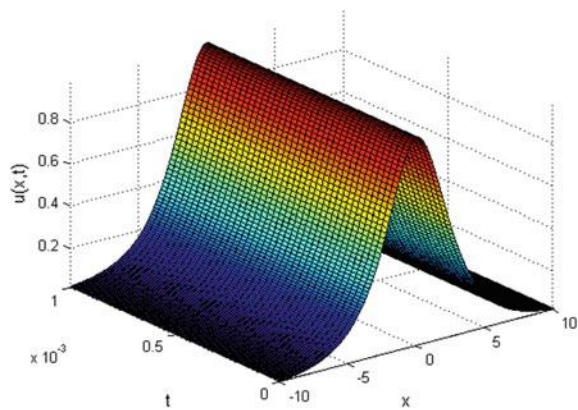
The choices of parameters  $a$  and  $b$  determine how well the waves propagate. When both Eqs. (2.2.9) and (2.3.2) are discretized in space with the fourth-order central difference scheme (2.1.13), it results in the ordinary differential equations in time. The resulting ODEs is advanced with the **MATLAB ode15s** solver.

To this end, we have dealt with spatial discretization method using finite difference (FD) schemes of higher orders. A less rigorous method of derivation of higher order FD schemes has been reported with the aid of a Mathematica program that contains the pre-loaded Padé package, with a view of circumventing the difficulty associated with the derivation of FD formula with order greater than two, see Tables 2.1 and 2.2 for details. Also, the question of ‘why using fourth-order FD schemes against the commonly used second-order scheme’ is well answered. A proof of this assertion is clearly shown in the results presented in Tables 2.3 and 2.4 for the second- and fourth-order FD schemes, respectively, for different values of  $\Delta x$ . It is evident from the results presented that the fourth-order scheme yields a better approximation in comparison to the second-order scheme, as the formal permits the use of higher step size. More importantly, the convergence test results presented in Fig. 2.1 further



**Fig. 2.1** Convergence of second-order (2.1.14) and fourth-order (2.1.13) central finite difference methods. The results presented here show the plots of maximum errors on the grid against  $N$ . The use of Toeplitz matrices allows high values of  $N$

**Fig. 2.2** Solution of the heat or diffusion equation (2.3.2) at parameters  $D = 0.5$ ,  $\delta = 0.5$ ,  $t = 0.001$ ,  $N = 200$  for  $x \in [-10, 10]$



justify the supremacy of fourth-order scheme (2.1.13) over its second-order counterpart (2.1.14) by error factor of about  $10^{-14}$  against  $10^{-7}$ , respectively. Accuracy and suitability of our schemes was ascertained via the analysis of their basic properties such as *order of accuracy*, *consistency*, *convergence*, *stability* and *symmetry* (Figs. 2.2 and 2.3).

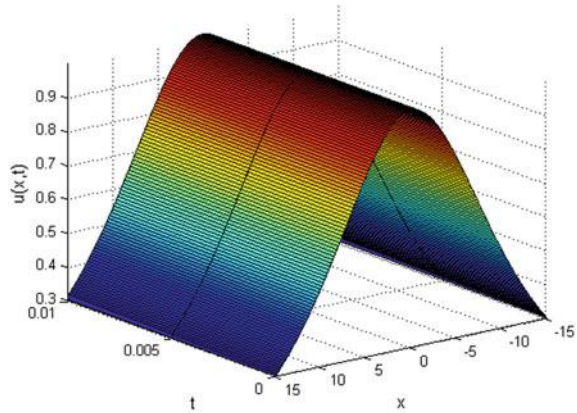
### 2.5 Finite Difference Approximations Schemes for Fractional Equations

In this chapter, we discuss the finite difference schemes for the fractional diffusion-advection equation

$$\frac{\partial u}{\partial t} = d \left( \frac{1}{2} + \frac{\gamma}{2} \right) \frac{\partial^\alpha u}{\partial x^\alpha} + d \left( \frac{1}{2} - \frac{\gamma}{2} \right) \frac{\partial^\alpha u}{\partial (-x)^\alpha} - Z \frac{\partial u}{\partial x}, \tag{2.5.1}$$

**Fig. 2.3** Solution of the heat or diffusion equation (2.2.9) at parameters

$D = 0.05$ ,  $\delta = 0.125$ ,  $\tau = 5$ ,  $\kappa = 1$ ,  $t = 0.01$ ,  $N = 200$  for  $x \in [-15, 15]$



where  $u$  is the resident solute concentration or sometimes referred as density,  $Z$  is the average pore-water velocity,  $x$  and  $t$  are the respective spatial and time coordinates,  $d$  stands for the diffusion coefficient,  $\alpha$  represents the order of the fractional differentiation with  $1 < \alpha \leq 2$ . The relative weight of solute particle forward versus backward transition probability is given by  $\gamma$  with  $-1 \leq \gamma \leq 0$ , which means that the transition probability is skewed backward, but if  $\gamma$  is bounded in the interval  $0 \leq \gamma \leq 1$ , we have the transition probability is skewed forward. If we define a fractional operator,  $\nabla_\gamma^\alpha$ , such as

$$2\nabla_\gamma^\alpha u = (1 + \gamma) \frac{\partial^\alpha u}{\partial x^\alpha} + (1 - \gamma) \frac{\partial^\alpha u}{\partial (-x)^\alpha}, \quad (2.5.2)$$

then, we can simply write (2.5.1) in the form

$$\frac{\partial u}{\partial t} + Z \frac{\partial u}{\partial x} = d \nabla_\gamma^\alpha u. \quad (2.5.3)$$

Apart from the from the fractional derivatives (Riemann–Liouville, Caputo and so on) emphasized in this book, another way of representing the fractional derivatives is by the Grünwald–Letnikov scheme, that is,

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x, t) = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x} \sum_{\tau=0}^{\lfloor \frac{x-a}{\Delta x} \rfloor} (-1)^\tau \binom{\alpha}{\tau} u(x - \tau \Delta x, t), \quad (2.5.4)$$

$$\frac{\partial^\alpha u}{\partial (-x)^\alpha}(x, t) = \lim_{\Delta x \rightarrow 0} \frac{1}{\Delta x^\alpha} \sum_{\tau=0}^{\lfloor \frac{b-x}{\Delta x} \rfloor} (-1)^\tau \binom{\alpha}{\tau} u(x - \tau \Delta x, t),$$

where  $\lfloor a \rfloor$  accounts for the integer part of  $a$ . Readers are referred to [17, 31, 34] for further properties about the fractional derivatives.

To determine the explicit schemes, we use a variant of the Grünwald–Letnikov method, in which the function evaluations are shifted to the left or right and we obtain what is known as the shifted Grünwald–Letnikov formula. The shift above corresponds to replacing the respective  $u(x - \tau \Delta x, t)$  and  $u(x + \tau \Delta x, t)$  by  $u(x - \tau \Delta x + \Delta x, t)$  and  $u(x + \tau \Delta x - \Delta x, t)$ , which does not affect the limit as  $\Delta x \rightarrow 0$ . The essence of choosing the shifted Grünwald–Letnikov formula is in two folds. The first reason is due to the way the generalizations of the existing schemes is obtained, that is, when the fractional-order  $\alpha = 2$ , we recall the standard advection diffusion equation. The second reason is due to the fact that the approximations of the derivatives obtained by using the classical Grünwald–Letnikov method very frequently originate unstable numerical schemes, see, for example, [24, 39].

It should be mentioned that some of the numerical schemes reported in the literature for this type of problems are implicit, but explicit schemes are easier to implement, and can be considered as most appropriate for such transient problems. We present a more general explicit scheme here for the advection diffusion equation.

To derive a fractional finite difference scheme we assume there are approximations  $\mathbf{U} = \{U_j^n\}$  to the values  $U(x_j, t_n)$  at the mesh points

$$x_j = j \Delta x, \quad j = -N, \dots, -2, -1, 0, 1, 2, \dots, N \quad \text{and} \quad t_n = n \Delta t, \quad n \geq 0,$$

where  $\Delta x$  represents the uniform space step and  $\Delta t$  stands for the uniform time step. For the uniform space step  $\Delta x$  and time step  $\Delta t$ , we let

$$\nu = \frac{Z \Delta t}{\Delta x} \quad \text{and} \quad \omega_\alpha = \frac{d \Delta t}{\Delta x^\alpha}.$$

here, the quantity  $\nu$  is known as the Courant–Friedrichs–Lewy (CFL) number, and parameter  $\omega$  is associated with the diffusion coefficient.

The finite difference schemes will be described based on the upwind, central and second difference operators, define, respectively, as [39]

$$\Delta_- U_j^n = U_j^n - U_{j-1}^n, \quad \Delta_0 U_j^n = \frac{U_{j+1}^n - U_{j-1}^n}{2}, \quad \text{and} \quad \xi^2 U_j^n = U_{j+1}^n - 2U_j^n + U_{j-1}^n.$$

We define a discrete approximation to the fractional derivative terms from the shifted Grünwald–Letnikov formulas as

$$\begin{aligned} \left( \frac{\partial^\alpha u}{\partial x^\alpha} \right)_j^n &\simeq \frac{1}{\Delta x^\alpha} \sum_{\tau=0}^{N+j+1} p_\tau U_{j+1-\tau}^n, \\ \left( \frac{\partial^\alpha u}{\partial (-x)^\alpha} \right)_j^n &\simeq \frac{1}{\Delta x^\alpha} \sum_{\tau=0}^{N-j+1} p_\tau U_{j-1+\tau}^n, \end{aligned} \tag{2.5.5}$$

for

$$p_\tau = (-1)^\tau \binom{\alpha}{\tau} = (-1)^\tau \frac{\alpha(\alpha-1)\cdots(\alpha-\tau+1)}{\tau!} = \frac{\Gamma(\tau-\alpha)}{\Gamma(-\alpha)\Gamma(\tau+1)}. \quad (2.5.6)$$

The fractional operator  $\nabla_\gamma^\alpha$ , given by (2.5.2), is approximated by  $\xi_\gamma^\alpha/2\Delta x^\alpha$  where  $\xi_\gamma^\alpha$  is defined by

$$\xi_\gamma^\alpha U_j^n = (1+\gamma) \sum_{\tau=0}^{N+j+1} p_\tau U_{j+1-\tau}^n + (1-\gamma) \sum_{\tau=0}^{N-j+1} p_\tau U_{j-1+\tau}^n. \quad (2.5.7)$$

Therefore, we write the finite difference scheme for the approximation of (2.5.1) in the form

$$U_j^{n+1} = U_j^n - v\Delta_- U_j^n + \frac{1}{2}\omega_\alpha \xi_\gamma^\alpha U_j^n. \quad (2.5.8)$$

According to the discretization of the advective, we call the above scheme the central difference scheme. Another approximation is obtained by replacing the upwind operator with the central operator, in the form,

$$U_j^{n+1} = U_j^n - v\Delta_0 U_j^n + \frac{1}{2}\omega_\alpha \xi_\gamma^\alpha U_j^n. \quad (2.5.9)$$

The last scheme is derived in a similar way to the Lax–Wendroff scheme [22]. If  $u$  is expanded around the time level  $n$ , we get

$$u^{n+1} = u^n + \Delta_t \frac{\partial u^n}{\partial t} + \frac{\Delta t^2}{2} \frac{\partial^2 u^n}{\partial t^2} + \mathcal{O}(\Delta t^3). \quad (2.5.10)$$

From (2.5.3), and with  $d = 0$ , we obtain

$$\frac{\partial^2 u}{\partial t^2} = Z^2 \frac{\partial^2 u}{\partial x^2}. \quad (2.5.11)$$

By putting (2.5.3) and (2.5.11) into (2.5.10) yields

$$U_j^{n+1} = U_j^n + \Delta_t \left[ -Z \left( \frac{\partial u}{\partial x} \right)_j^n + d(\nabla_\gamma^\alpha u)_j^n \right] + \frac{\Delta t^2}{2} Z^2 \left( \frac{\partial^2 u}{\partial x^2} \right)_j^n.$$

Hence, the Lax–Wendroff scheme can be written in the form

$$U_j^{n+1} = U_j^n - z\Delta_0 U_j^n + \frac{\omega_\alpha \xi_\gamma^\alpha U_j^n}{2} + \frac{z^2 \xi^2 U_j^n}{2}. \quad (2.5.12)$$

### 2.5.1 Matrix Representation of the Finite Difference Schemes

In this section, we want to write the above explicit schemes in matrix form. Suppose that the nodal points are  $U_j^n = -N, \dots, -2, -1, 0, 1, 2, \dots, N$ , assume also that the boundary conditions are known, that is, from the functions  $U_{-N}^n$  and  $U_N^n$  for  $n = 0, 1, 2, \dots$ .

By introducing the vector  $\mathbf{U}^n = [U_{-N+1}^n, \dots, U_{-1}^n, U_0^n, U_1^n, U_2^n, \dots, U_{N-1}^n]^T$ , we can write the schemes as matrix equation

$$\mathbf{U}^{n+1} = \mathbf{G}\mathbf{U}^n + \mathbf{z}^n, \quad n = 0, 1, 2, \dots, \quad (2.5.13)$$

where  $\mathbf{G}$  is the matrix iteration of size  $(2N - 1) \times (2N - 1)$ , and  $\mathbf{z}^n$  is the vector containing the boundary values.

The matrix  $\mathbf{G}$  can be written as

$$\mathbf{G} = \mathbf{A} + \frac{1}{2}\omega_\alpha \mathbf{B}, \quad (2.5.14)$$

where  $\mathbf{A}$  and  $\mathbf{B}$  are matrices of equal dimension  $(2N - 1) \times (2N - 1)$  and  $\mathbf{A}$  corresponds to the advection discretization while  $\mathbf{B}$  is related with the diffusion discretization.

For all the schemes discussed above, the matrix  $\mathbf{B}$  is the same and is defined by

$$\mathbf{B} = (1 + \gamma)\mathbf{L} + (1 - \gamma)\mathbf{L}^T,$$

where

$$\mathbf{L} = \begin{pmatrix} p_1 & p_0 & 0 & \cdots & 0 \\ p_2 & & & & \\ & & \ddots & & \vdots \\ & & & \ddots & 0 \\ & & & & p_0 \\ p_{2N-1} & \cdots & p_2 & p_1 \end{pmatrix}. \quad (2.5.15)$$

The vector  $\mathbf{z}^n$  has two parts

$$\mathbf{z}^n = \mathbf{z}_\mathbf{A}^n + \mathbf{z}_\mathbf{B}^n,$$

where the vector  $\mathbf{z}_\mathbf{A}^n$  contains the boundary values that correspond to the matrix  $\mathbf{A}$  and the vector  $\mathbf{z}_\mathbf{B}^n$  has the boundary values relating to the matrix  $\mathbf{B}$ . For  $\mathbf{z}_\mathbf{B}^n$ , we have

$$\mathbf{z}_\mathbf{B}^n = \mathbf{z}_{B+}^n + \mathbf{z}_{B-}^n,$$

where

$$\mathbf{z}_{B+}^n = \frac{\omega_\alpha(1+\gamma)}{2} \begin{pmatrix} p_2 \\ \vdots \\ p_{2N-1} \\ p_{2N} \end{pmatrix} U_{-N}^n + \frac{\omega_\alpha(1+\gamma)}{2} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ p_{2N} \end{pmatrix} U_N^n$$

and

$$\mathbf{z}_{B-}^n = \frac{\omega_\alpha(1-\gamma)}{2} \begin{pmatrix} p_0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} U_{-N}^n + \frac{\omega_\alpha(1-\gamma)}{2} \begin{pmatrix} p_{2N} \\ p_{2N-1} \\ \vdots \\ p_2 \end{pmatrix} U_N^n.$$

For the upwind scheme the matrix  $\mathbf{A}$  and the vector  $\mathbf{z}_A^n$  are, respectively, given as

$$\mathbf{A}_* = \begin{pmatrix} 1-z & & & \\ & z & \ddots & \\ & & \ddots & \\ & & & z & 1-z \end{pmatrix} \quad \text{and} \quad \mathbf{z}_*^n = \begin{pmatrix} z \\ 0 \\ \vdots \\ 0 \end{pmatrix} U_{-N}^n.$$

For the central difference scheme, the matrix  $\mathbf{A}$  and the vector  $\mathbf{z}_A^n$  are, respectively, given as

$$\mathbf{A}_{**} = \begin{pmatrix} 1 & -z/2 & & \\ z/2 & \ddots & \ddots & \\ & \ddots & & -z/2 \\ & & z/2 & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{z}_{**}^n = \begin{pmatrix} z/2 \\ 0 \\ \vdots \\ 0 \end{pmatrix} U_{-N}^n + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ -z/2 \end{pmatrix} U_N^n.$$

For the Lax–Wendroff scheme, the matrix  $\mathbf{A}$  and the vector  $\mathbf{z}_A^n$  are, respectively, given as

$$\mathbf{A}_{***} = \begin{pmatrix} 1-z^2 & \frac{z(z-1)}{2} & & \\ \frac{z(z+1)}{2} & & \ddots & \\ & \ddots & & \frac{z(z-1)}{2} \\ \frac{z(z+1)}{2} & & & 1-z^2 \end{pmatrix}$$

and

$$\mathbf{z}_{***}^n = \begin{pmatrix} \frac{z(z+1)}{2} \\ \vdots \\ 0 \\ 0 \end{pmatrix} U_{-N}^n + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \frac{z(z-1)}{2} \end{pmatrix} U_N^n.$$

## 2.5.2 Convergence Analysis of Fractional Finite Difference Schemes

Convergence of the finite difference schemes is considered in this section. We first show that the schemes are consistent with Eq. (2.5.1), and second examine under which conditions they are stable. We adopt two methods for the stability analysis.

### 2.5.2.1 Consistency

For the numerical schemes presented above, we analyse the truncation error  $T_j^n$ . We assume  $u = u(x, t)$  to be the solution of our equation. In the schemes, we approximate the fractional operator  $\nabla_\gamma^\alpha$  by  $\frac{\xi_\beta^\alpha}{2\Delta x^\alpha}$ . According to Meerschaert and Tadjeran [24], this operator is first-order accurate for the case of homogeneous boundary conditions, that is

$$\frac{\xi_\beta^\alpha u_j^n}{2\Delta x^\alpha} = (\Delta_\gamma^\alpha u)_j^n + \mathcal{O}(\Delta x).$$

By using this result for the upwind scheme, we obtain

$$\begin{aligned} T_j^n &= \frac{u_j^{n+1} - u_j^n}{\Delta t} + Z \frac{u_j^n - u_{j-1}^n}{\Delta x} - \frac{d}{2\Delta x^\alpha} \xi_\gamma^\alpha u_j^n \\ &= \left( \frac{\partial u}{\partial t} \right)_j^n + \mathcal{O}(\Delta t) + Z \left( \frac{\partial u}{\partial x} \right)_j^n + \mathcal{O}(\Delta x) - d(\Delta_\gamma^\alpha u)_j^n + \mathcal{O}(\Delta x). \end{aligned}$$

We therefore say that the upwind scheme has an order of accuracy  $\mathcal{O}(\Delta t) + \mathcal{O}(\Delta x) + \mathcal{O}(\Delta x)$ .

Similarly for the central scheme, we get

$$\begin{aligned} T_j^n &= \frac{u_j^{n+1} - u_j^n}{\Delta t} + Z \frac{u_j^{n+1} - u_{j-1}^n}{2\Delta x} - \frac{d}{2\Delta x^\alpha} \xi_\gamma^\alpha u_j^n \\ &= \left( \frac{\partial u}{\partial t} \right)_j^n + \mathcal{O}(\Delta t) + Z \left( \frac{\partial u}{\partial x} \right)_j^n + \mathcal{O}(\Delta x^2) - d(\Delta_\gamma^\alpha u)_j^n + \mathcal{O}(\Delta x), \end{aligned}$$

with the order of accuracy  $\mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta x)$ .

For the Lax–Wendroff scheme, we obtain

$$\begin{aligned} T_j^n &= \frac{u_j^{n+1} - u_j^n}{\Delta t} + Z \frac{u_j^{n+1} - u_{j-1}^n}{2\Delta x} - Z^2 \frac{\Delta t}{2} \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta x^2} - \frac{d}{2\Delta x^\alpha} \xi_\gamma^\alpha u_j^n \\ &= \left( \frac{\partial u}{\partial t} \right)_j^n + \frac{\Delta t}{2} \left( \frac{\partial^2 u}{\partial t^2} \right)_j^n + \mathcal{O}(\Delta t^2) + Z \left( \frac{\partial u}{\partial x} \right)_j^n + \mathcal{O}(\Delta x^2) - Z^2 \frac{\Delta t}{2} \left( \frac{\partial^2 u}{\partial x^2} \right)_j^n \\ &\quad + \mathcal{O}(\Delta x^2) - d(\Delta_\gamma^\alpha u)_j^n + \mathcal{O}(\Delta x). \end{aligned}$$

The order of accuracy is  $\mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta x)$ . For small value of  $d$ , it follows from (2.5.11) that

$$T_j^n = \left( \frac{\partial u}{\partial t} \right)_j^n + \mathcal{O}(\Delta t^2) + Z \left( \frac{\partial u}{\partial x} \right)_j^n + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta x^2) - d(\Delta \gamma^\alpha u)_j^n + \mathcal{O}(\Delta x),$$

and the Lax–Wendroff scheme has an order of accuracy close to  $\mathcal{O}(\Delta t^2) + \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta x)$ .

### 2.5.3 Stability Analysis of Fractional Finite Difference Schemes

In attempt to obtain necessary stability conditions for the fractional finite difference schemes, we adopt the Fourier analysis or von Neumann analysis, as in the classical case. Moreover, we derive sufficient stability conditions obtained by computing numerically the norm of the matrix iteration of each scheme. These conditions permit us to conclude that some of the theoretical necessary conditions obtained with the von Neumann analysis are necessary and sufficient conditions for stability. Fourier or von Neumann analysis assumes that we have a solution defined in the whole real line. It is also applied to problems with periodic boundary conditions since the solution is considered as a periodic function bounded in  $\mathbb{R}$ . Although von Neumann analysis gives necessary and sufficient stability conditions only when applied to pure initial value problems and to problems with periodic boundary conditions, it is certain that the von Neumann technique always gives necessary conditions for stability whether the problem boundary conditions is periodic or not.

The von Neumann analysis takes an assumption that any finite mesh function, for instance, the numerical solution  $U_j^n$  has tendency to decompose into a Fourier series in the form

$$U_j^n = \sum_{s=-N}^N \varphi_s^n e^{i\kappa_s(j\Delta x)}, \quad j = -N, \dots, N,$$

where  $\varphi_s^n$  denotes the amplitude of the  $s$ th harmonic, and  $\kappa_s = \frac{s\pi}{N\Delta x}$ . The product  $\kappa\Delta x$  is sometimes referred to as the phase angle  $\eta = \kappa_s\Delta x$  which covers the entire domain  $[-\pi, \pi]$  in steps of  $\pi/N$ .

If the amplitude factor  $\varphi$  does not grow in time, then the stability conditions will be satisfied, that is, if we have  $|\varphi(\eta)| \leq 1$ , for all  $\eta$ . At first, we provide some straightforward properties related to the coefficients  $p_\tau$ ,  $\tau = 0, 1, \dots, 2N$ .

**Proposition 2.5.1** *The coefficients  $p_\tau$ ,  $\tau = 0, 1, \dots, 2N$  hold for: (a)  $p_0 = 1$ ,  $p_1 = -\alpha$ ,  $p_2 = \frac{\alpha(\alpha-1)}{2}$  and  $p_\tau > 0$ , for  $\tau \geq 3$ . (b)  $\sum_{\tau=2}^{\infty} p_\tau = \alpha - 1$ .*

*Proof* (a) We are permitted to write  $p_\tau$  as

$$p_0 = 1 \quad \text{and} \quad p_{\tau+1} = -\frac{(\alpha - \tau)}{\tau + 1} p_\tau, \quad \tau \geq 1.$$

Specifically, we have  $p_1 = -\alpha$  and  $p_2 = \frac{\alpha(\alpha-1)}{2} > 0$ . Since  $\alpha - \tau < 0$  for  $\tau \geq 3$ , by induction we conclude that  $p_\tau > 0$  for  $\tau \geq 3$ . (b) This second part result follows directly from  $\sum_{\tau=0}^{\infty} p_\tau = 0$ , since  $p_0 + p_1 + \sum_{\tau=2}^{\infty} p_\tau = 0$  for  $p_0 = 1$  and  $p_1 = -\alpha$ .  $\square$

With  $Z = 0$ , Eq. (2.5.1) reduces to fractional diffusion equation

$$U_j^{n+1} = U_j^n + \frac{\omega_\alpha \xi_\gamma^\alpha U_j^n}{2}. \quad (2.5.16)$$

To adopt the von Neumann analysis, we first assume that the problem is defined in  $\mathbb{R}$  and therefore define the discrete operator  $\xi_\gamma^\alpha$  by

$$\xi_\gamma^\alpha U_j^n = (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau U_{j+1-\tau}^n + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau U_{j-1+\tau}^n. \quad (2.5.17)$$

Hence, we can write scheme (2.5.16) in the form

$$U_j^{n+1} = U_j^n + \frac{\omega_\alpha}{2} \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau U_{j+1-\tau}^n + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau U_{j-1+\tau}^n \right\}. \quad (2.5.18)$$

It should be noted that when  $\alpha = 2$ , we have  $p_0 = 1$ ,  $p_1 = -2$ ,  $p_2 = 1$  and  $p_\tau = 0$  for all  $\tau \geq 3$ .

**Theorem 2.5.2** *Let  $-1 \leq \gamma \leq 1$  and  $1 < \alpha \leq 2$ . If numerical scheme (2.5.18) is von Neumann stable, then  $\omega_\alpha \leq 2^{1-\alpha}$ .*

*Proof* By putting mode  $\varphi^n e^{ij\eta}$  into (2.5.18), we obtain the amplification factor

$$\varphi(\eta) = 1 + \frac{\omega_\alpha}{2} \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau e^{i(1-\tau)\eta} + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau e^{-i(1-\tau)\eta} \right\}. \quad (2.5.19)$$

Next, we consider the cases  $\eta = 0$  and  $\eta = \pi$  in Eq. (2.5.19). Bear in mind that the region around  $\eta = 0$  and  $\eta = \pi$  corresponds to the low and high frequencies, respectively.

So, for  $\eta = 0$  the amplification factor (2.5.19) reduces to

$$\varphi(0) = 1 + \frac{\omega_\alpha}{2} \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau \right\},$$

since  $\sum_{\tau=0}^{\infty} p_\tau = 0$  then  $\varphi(0) = 1$ .

For  $\eta = \pi$ , the amplification factor (2.5.19) becomes

$$\varphi(\pi) = 1 + \frac{\omega_\alpha}{2} \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau \cos((1 - \tau)\pi) + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau \cos((1 - \tau)\pi) \right\}.$$

Since  $\cos((1 - \tau)\pi) = (-1)^{\tau-1}$ , it directly follows that

$$\begin{aligned} \varphi(\pi) &= 1 + \frac{\omega_\alpha}{2} \left\{ -(1 + \gamma) \sum_{\tau=0}^{\infty} \sigma_\tau + (1 - \gamma) \sum_{\tau=0}^{\infty} \sigma_\tau \right\} \\ &= 1 - \omega_\alpha \sum_{\tau=0}^{\infty} \sigma_\tau, \end{aligned}$$

where  $\sigma_\tau = \binom{\alpha}{\tau}$ , and the condition  $|\varphi(\pi)| \leq 1$  has equivalence

$$\omega_\alpha \sum_{\tau=0}^{\infty} \sigma_\tau \leq 2.$$

Therefore, we conclude that for  $\sum_{\tau=0}^{\infty} \sigma_\tau = 2^\alpha$ , we must have  $\omega_\alpha 2^\alpha \leq 2$ , that is,  $\omega_\alpha \leq 2^{1-\alpha}$ .  $\square$

The next stability result is for the upwind scheme (2.5.8).

**Theorem 2.5.3** *Let  $-1 \leq \gamma \leq 1$  and  $1 < \alpha \leq 2$ . If the upwind scheme (2.5.8) is von Neumann stable, then  $z + \omega_\alpha 2^{\alpha-1} \leq 1$ .*

*Proof* The amplification factor for the upwind scheme is given by

$$\varphi_U(\eta) = 1 - z(1 - e^{-i\eta}) + \frac{\omega_\alpha}{2} \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau e^{i(1-\tau)\eta} + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau e^{-i(1-\tau)\eta} \right\}.$$

For  $\eta = \pi$ , it follows that:

$$\varphi_U(\pi) = 1 - 2z - \frac{\omega_\alpha}{2} \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} \sigma_\tau + (1 - \gamma) \sum_{\tau=0}^{\infty} \sigma_\tau \right\}.$$

For condition  $|\varphi_U(\pi)| \leq 1$  to be satisfied, we must have

$$2z + \omega_\alpha \sum_{\tau=0}^{\infty} \sigma_\tau \leq 2.$$

Moreover

$$2z + \omega_\alpha \sum_{\tau=0}^{\infty} \sigma_\tau = 2z + \omega_\alpha 2^\alpha$$

and  $2z + \omega_\alpha 2^\alpha \leq 2$  shows that  $z + \omega_\alpha 2^{\alpha-1} \leq 1$ . This completes the proof.  $\square$

The following stability result is for the Lax–Wendroff scheme (2.5.12).

**Theorem 2.5.4** *Let  $-1 \leq \gamma \leq 1$  and  $1 < \alpha \leq 2$ . If the Lax–Wendroff scheme (2.5.8) is von Neumann stable, then  $z^2 + \omega_\alpha 2^{\alpha-1} \leq 1$ .*

*Proof* The above result is similar to that of the upwind scheme. The amplification factor for the Lax–Wendroff scheme (2.5.12) takes the form

$$\begin{aligned} \varphi_L(\eta) = & 1 - \frac{z}{2}(e^{i\eta} - e^{-i\eta}) + \frac{z^2}{2}(e^{i\eta} - 2 + e^{-i\eta}) \\ & + \frac{1}{2}\omega_\alpha \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau e^{i(1-\tau)\eta} + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau e^{-i(1-\tau)\eta} \right\}. \end{aligned}$$

For  $\eta = \pi$ , we obtain

$$\varphi_L(\pi) = 1 - 2z^2 - \frac{1}{2}\omega_\alpha \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau \right\}.$$

Also for condition  $|\varphi_L(\pi)| \leq 1$  to be satisfied, we must have

$$2z^2 + \omega_\alpha \sum_{\tau=0}^{\infty} \sigma_\tau \leq 2.$$

Moreover

$$2z^2 + \omega_\alpha \sum_{\tau=0}^{\infty} \sigma_\tau = 2z^2 + \omega_\alpha 2^\alpha$$

and  $2z^2 + \omega_\alpha 2^\alpha \leq 2$  shows that  $z^2 + \omega_\alpha 2^{\alpha-1} \leq 1$ . The proof is completed.  $\square$

Obviously, derivation of stability conditions for the central scheme is much more difficult than for the previous schemes. For the central scheme of the standard advection diffusion equation, that is, for  $\alpha = 2$ , it was also hard. In fact, the stability analysis reported for this scheme over the years was found controversial due to the

apparent difficulty of obtaining stability conditions, see, for example, [38, 39]. The following theorem relating to the central scheme maps out necessary stability conditions. These conditions are not as strong as the necessary conditions of the previous theorems given in this chapter, in the sense that they are less close to the respective necessary and sufficient stability conditions, as we shall see in this book.

**Theorem 2.5.5** *Let  $-1 \leq \gamma \leq 1$  and  $1 < \alpha \leq 2$ . If the central scheme (2.5.9) is von Neumann stable, then  $\omega_\alpha 2^{\alpha-1} \leq 1$ .*

*Proof* For the central scheme (2.5.9), the amplification factor is written as

$$\varphi_C(\eta) = 1 - \frac{z}{2}(e^{i\eta} - e^{-i\eta}) + \frac{1}{2}\omega_\alpha \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau e^{i(1-\tau)\eta} + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau e^{-i(1-\tau)\eta} \right\}.$$

For  $\eta = \pi$ , we get

$$\varphi_C(\pi) = 1 - \frac{1}{2}\omega_\alpha \left\{ (1 + \gamma) \sum_{\tau=0}^{\infty} p_\tau + (1 - \gamma) \sum_{\tau=0}^{\infty} p_\tau \right\}$$

and from previous result, we already know that  $|\varphi_C(\pi)| \leq 1$ , which implies that  $\omega_\alpha \leq 2^{1-\alpha}$ . □

## 2.6 Numerical Approximation of Time-Fractional Sub-diffusion Process with the Second-Order Implicit Difference Method

In this section, we seek implicit difference approximations for the time-fractional sub-diffusion order process. We show that when the solution of the sub-diffusion equation is a sufficiently differentiable function the difference approximations have second-order accuracy  $\mathcal{O}(k^2 + h^2)$ . The theoretical solution of the time-fractional sub-diffusion problem can be found by using the Laplace–Fourier transform [4, 31] or separation of variables for special cases of the boundary conditions and the function  $F(x, t)$ . The time-fractional diffusion equation

$$\left. \begin{aligned} \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} &= \frac{\partial^2 u(x, t)}{\partial x^2}, \\ u(0, t) = u(1, t) &= 0, \quad u(x, 0) = \psi(x) \end{aligned} \right\} \tag{2.6.1}$$

has an exact solution of the form

$$u(x, t) = 2 \sum_{n=1}^{\infty} \nu_n E_\alpha(-n^2 \pi^2 t^\alpha) \sin(n\pi x) \tag{2.6.2}$$

on the domain  $\{0 \leq x \leq 1, t \geq 0\}$ , where

$$\nu_n = \int_0^1 \psi(\tau) \sin(n\pi\tau) d\tau$$

and  $E_\alpha$  denotes the one-parameter Mittag–Leffler function as defined in the previous chapter. Each term

$$E_\alpha(-n^2\pi^2t^\alpha) \sin(n\pi x)$$

is assumed to be a solution of (2.6.1) and  $\nu_n$  is the coefficient of the Fourier sine series of the function  $\psi(x)$ .

### 2.6.1 Second-Order Implicit Difference Approximation

When the order of the fractional derivative lies between zero and one (that is,  $0 < \alpha < 1$ ), such equation is referred to as the fractional sub-diffusion equation. The fractional sub-diffusion equation is known to be an important equation in fractional calculus. The implicit difference approximation which utilizes the quadrature approximation in the form

$$u_n^{(\alpha)} = \frac{1}{h^\alpha} \sum_{s=0}^{n-1} \nu_k^{(\alpha)} u_{n-s} + \mathcal{O}(h^{2-\alpha})$$

with  $\nu_0^{(\alpha)} = 1/\Gamma(2-\alpha)$  and

$$\nu_s^{(\alpha)} = \frac{(s+1)^{1-\alpha} - 2s^{1-\alpha} + (s-1)^{1-\alpha}}{\Gamma(2-\alpha)}$$

for the fractional derivative and central difference approximation technique for the second-order spatial derivative with respect to  $x$ , has accuracy  $\mathcal{O}(k^2 + h^2)$  [11]. Finite difference approximations are easier and much more convenient way to approximate the solution of PDEs. They combine simple description with stability and high accuracy. Even when the analytical solution of the time-fractional diffusion equation is available, the finite difference approximations may possess higher accuracy than approximations using the exact solution.

The approximation error of a numerical solution of Eq. (2.6.1) approximated by truncating (2.6.2) contains errors from the truncation of the Fourier series at the end-points and the approximations of the coefficients  $\nu_n$  and the Mittag–Leffler functions. In this chapter, we find second-order difference approximations for Eq. (2.6.1) on the computational domain size

$$L = [0, 1] \times [0, T].$$

By adding the function  $F(x, t)$  to the right-hand side of (2.6.1), we assume that it has homogeneous initial and boundary conditions

$$\left. \begin{aligned} \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} &= \frac{\partial^2 u(x, t)}{\partial x^2} + F(x, t), \\ u(0, t) = u(1, t) &= 0, \quad u(x, 0) = 0. \end{aligned} \right\} \tag{2.6.3}$$

So, if (2.6.1) is given with either nonhomogeneous initial or boundary conditions, the substitution

$$\bar{u}(x, t) = u(x, t) - u(x, 0) - (1 - x)(u(0, t)) - u(0, 0) - x(u(1, t) - u(1, 0))$$

changes the equation to the type which has the same form of homogeneous initial and boundary conditions.

Before proceeding, the following lemma briefly discusses a property of the Caputo derivative of a continuously differentiable function in the neighbourhood of the lower limit  $a$ .

**Lemma 2.6.1** *Given the ordinary fractional differential equation*

$$u^{(\alpha)}(x) + u(x) = f(x). \tag{2.6.4}$$

Let  $0 < \alpha < 1$  and  $u \in C^1[a, a + \epsilon]$ , where  $\epsilon > 0$ . Then

$$u^{(\alpha)}(a) = 0.$$

*Proof* The function  $u'$  is bounded on the interval  $[a, a + \epsilon]$ . Assume

$$\delta = \max_{a \leq x \leq a + \epsilon} u'(x).$$

When  $a < x < a + \epsilon$ , we have

$$\begin{aligned} |u^{(\alpha)}(x)| &\leq \frac{1}{\Gamma(1 - \alpha)} \int_a^x \frac{|u'(\tau)|}{(x - \tau)^\alpha} d\tau \\ &\leq \frac{\delta}{\Gamma(1 - \alpha)} \int_a^x (x - \tau)^{-\alpha} d\tau, \\ |u^{(\alpha)}(x)| &\leq \frac{\delta}{\Gamma(1 - \alpha)} - \frac{(x - \tau)^{1-\alpha}}{1 - \alpha} \Big|_a^x \leq \frac{\delta(x - a)^{1-\alpha}}{\Gamma(2 - \alpha)}. \end{aligned} \tag{2.6.5}$$

From the squeeze law of limits, we have

$$0 \leq \lim_{x \downarrow a} |u^{(\alpha)}(x)| \leq \lim_{x \downarrow a} \frac{\delta(x - a)^{1-\alpha}}{\Gamma(2 - \alpha)} = 0.$$

Hence,

$$u^{(\alpha)}(a) = \lim_{x \downarrow a} u^{(\alpha)}(x) = 0.$$

□

In Lemma 2.6.1, we have proved that when the solution  $u(x, t)$  is sufficiently differentiable function w.r.t. the time variable  $t$ , the fractional derivative  $\frac{\partial^\alpha u(x, 0)}{\partial t^\alpha} \rightarrow 0$  when  $t = 0$ . If the solution  $u(x, t)$  has continuous second derivative, that is  $u_{xx}(x, t)$  w.r.t.  $t$ , then the function  $F(x, t)$  holds for the condition  $F(x, 0) = 0$ , which implies that

$$F(x, 0) = \left. \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} \right|_{t=0} - \left. \frac{\partial^2 u(x, t)}{\partial x^2} \right|_{t=0} = 0.$$

The above compatibility condition corresponds to the condition  $f(0) = 0$  for differentiable solution of ordinary fractional differential equation (2.6.4), subject to the initial condition  $u(0) = 0$ . In effort to formulate a second-order difference approximations for Eq. (2.6.1) using numerical approximation

$$u^{(\alpha)} \left\{ x - \frac{\alpha h}{2} \right\} = \frac{1}{h^\alpha} \sum_{n=0}^{N_{x,h}} \varphi_n^{(\alpha)} u(x - nh) + \mathcal{O}(h^2), \quad (2.6.6)$$

where

$$\frac{1}{h^\alpha} \sum_{n=0}^{N_{x,h}} \varphi_n^{(\alpha)} u(x - nh) = \left( \frac{\alpha}{2} \right) u_{n-1}^{(\alpha)} + \left( 1 - \frac{\alpha}{2} \right) u_n^{(\alpha)} + \mathcal{O}(h^2) \quad (2.6.7)$$

for the Caputo derivative, we first ensure that the first and second derivatives of the solution  $u_t(x, t)$  and  $u_{tt}(x, t)$  w.r.t. the time variable  $t$  are equal to zero when  $t = 0$ . Let

$$A_1(x) = \left. \frac{\partial u(x, t)}{\partial t} \right|_{t=0}, \quad A_2(x) = \left. \frac{\partial^2 u(x, 0)}{\partial t^2} \right|_{t=0} \quad \text{and} \quad A_3(x) = \left. \frac{\partial^3 u(x, 0)}{\partial t \partial x^2} \right|_{t=0}.$$

By applying time-fractional derivative of order  $1 - \alpha$  to (2.6.3), we have

$$\frac{\partial u(x, t)}{\partial t} = \frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} + \frac{\partial^{1-\alpha} F(x, t)}{t^{1-\alpha}}. \quad (2.6.8)$$

When  $u_{xx}(x, t)$  is bounded in  $\mathcal{D}$ , we have that  $\frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} = 0$ . Then

$$A_1(x) = \left. \frac{\partial^{1-\alpha} F(x, t)}{t^{1-\alpha}} \right|_{t=0}. \quad (2.6.9)$$

Next, Eq. (2.6.8) is differentiated w.r.t.  $t$  to obtain

$$\frac{\partial^2 u(x, t)}{\partial t^2} = \frac{\partial}{\partial t} \frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} + \frac{\partial}{\partial t} \frac{\partial^{1-\alpha} F(x, t)}{t^{1-\alpha}}. \quad (2.6.10)$$

The Caputo derivative of order  $1 - \alpha$  of the function  $u_{xx}(x, t)$  w.r.t.  $t$  is defined as

$$\frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} = \frac{t^{\alpha-1}}{\Gamma(\alpha)} \frac{\partial^3 u(x, t)}{\partial t \partial x^2} \Big|_{t=0} + \frac{1}{\Gamma(\alpha)} \int_0^t \frac{\partial^4 u(x, \tau)}{\partial t^2 \partial x^2} (t - \tau)^{\alpha-1} d\tau.$$

Considering the definition of the Caputo derivative of order  $2 - \alpha$  w.r.t.  $t$ , we have

$$\frac{1}{\Gamma(\alpha)} \int_0^t \frac{\partial^4 u(x, \tau)}{\partial t^2 \partial x^2} (t - \tau)^{\alpha-1} d\tau = \mathcal{D}_t^{2-\alpha} \frac{\partial^2 u(x, t)}{\partial x^2}.$$

So that

$$\frac{\partial^{3-\alpha} u(x, t)}{\partial t^{1-\alpha} \partial x^2} = \frac{t^{\alpha-1}}{\Gamma(\alpha)} A_3(x) + \mathcal{D}_t^{2-\alpha} \frac{\partial^2 u(x, t)}{\partial x^2}. \quad (2.6.11)$$

We have that

$$\frac{\partial^3 u(x, t)}{\partial t \partial x^2} = \frac{\partial}{\partial t} \left( \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} - F(x, t) \right) = \frac{\partial}{\partial t} \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} - \frac{\partial}{\partial t} F(x, t).$$

First integrate by parts and differentiate w.r.t.  $t$  to have

$$\frac{\partial}{\partial t} \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} = \frac{\partial u(x, t)}{\partial t} \frac{t^{-\alpha}}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial^2 u(x, \tau)}{\partial t^2} (t - \tau)^\alpha d\tau.$$

Then

$$\begin{aligned} \frac{\partial^3 u(x, t)}{\partial t \partial x^2} &= \frac{\partial u(x, t)}{\partial t} \frac{t^{-\alpha}}{\Gamma(1-\alpha)} + \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial^2 u(x, \tau)}{\partial t^2} (t - \tau)^\alpha d\tau - \frac{\partial}{\partial t} F(x, t), \\ &= \frac{A_1(x)}{\Gamma(1-\alpha)t^\alpha} + \mathcal{D}_t^{1-\alpha} u(x, t) - \frac{\partial}{\partial t} F(x, t). \end{aligned}$$

Hence, we compute the function  $A_3(x)$  as

$$A_3(x) = \frac{\partial^3 u(x, t)}{\partial t \partial x^2} \Big|_{t=0} = \lim_{t \downarrow 0} \left( \frac{A_1(x)}{\Gamma(1-\alpha)t^\alpha} - \frac{\partial}{\partial t} F(x, t) \right) \quad (2.6.12)$$

due to the fact that the Caputo derivative  $\mathcal{D}_t^{1+\alpha} u(x, 0) \rightarrow 0$  when  $u_{tt}(x, t)$  is bounded. From Eqs. (2.6.10) and (2.6.11), the function  $A_2(x)$  is computed, that is

$$\frac{\partial^2 u(x, t)}{\partial t^2} = \frac{t^{\alpha-1}}{\Gamma(\alpha)} A_3(x) + \mathcal{D}_t^{2-\alpha} \frac{\partial^2 u(x, t)}{\partial x^2} + \frac{\partial}{\partial t} \frac{\partial^{1-\alpha} F(x, t)}{t^{1-\alpha}},$$

$$A_2(x) = \frac{\partial^2 u(x, 0)}{\partial t^2} = \lim_{t \downarrow 0} \left( \frac{A_3(x)}{\Gamma(\alpha) t^{1-\alpha}} + \frac{\partial}{\partial t} \frac{\partial^{1-\alpha} F(x, t)}{t^{1-\alpha}} \right). \quad (2.6.13)$$

Let

$$\omega(x, t) = u(x, t) - A_1(x)t - \frac{A_2(x)}{2}t^2.$$

Note that the partial derivatives  $\omega_t(x, t)$  and  $\omega_{tt}(x, t)$  of the function  $\omega(x, t)$  are all equal to zero when  $t = 0$ , and

$$\frac{\partial^\alpha \omega(x, t)}{\partial t^\alpha} = \frac{\partial^\alpha u(x, t)}{\partial t^\alpha} - \frac{A_1(x)t^{1-\alpha}}{\Gamma(2-\alpha)} - \frac{A_2(x)t^{2-\alpha}}{\Gamma(3-\alpha)},$$

$$\frac{\partial^2 \omega(x, t)}{\partial t^2} = \frac{\partial^2 u(x, t)}{\partial t^2} - A_1''(x) - \frac{A_2''(x)}{2}t^2.$$

The function  $\omega(x, t)$  is considered as the solution of fractional sub-diffusion equation

$$\left. \begin{aligned} \frac{\partial^\alpha \omega(x, t)}{\partial t^\alpha} &= \frac{\partial^2 \omega(x, t)}{\partial x^2} + I(x, t), \\ \omega(0, t) &= \omega(1, t) = 0, \quad \omega(x, 0) = 0, \end{aligned} \right\} \quad (2.6.14)$$

where

$$I(x, t) = F(x, t) - \frac{A_1(x)t^{1-\alpha}}{\Gamma(2-\alpha)} - \frac{A_2(x)t^{2-\alpha}}{\Gamma(3-\alpha)} + A_1''(x) - \frac{A_2''(x)}{2}t^2. \quad (2.6.15)$$

In what follows, we now use (2.6.7) and a central difference approximation for  $u_{xx}(x, t)$  to design an implicit difference approximations (2.6.19) and (2.6.20) for Eq. (2.6.14).

**Theorem 2.6.2** (Dimitrov [4], Theorem 29) *Difference approximations (2.6.19) and (2.6.20) are unconditionally stable and converge to the solution of (2.6.14) with second-order accuracy w.r.t. the time and space variables.*

For Theorem 2.6.2, Dimitrov [4] have shown that the difference approximations are unconditionally stable and have second-order accuracy  $\mathcal{O}(k^2 + h^2)$ . Let  $h = 1/N$  and  $k = T/M$ , where both  $h$  and  $k$  are positive integers, and

$$x_n = nh, \quad t_m = mk, \quad \omega_n^m = \omega(x_n, t_m), \quad I_n^m = I(x_n, t_m).$$

Using approximation (2.6.7) and Eq. (2.6.14), we have

$$\begin{aligned}\Delta_h^\alpha \omega(x_n, t_m) &= \left(\frac{\alpha}{2}\right) \frac{\partial^\alpha \omega(x_n, t_{m-1})}{\partial t^\alpha} + \left(1 - \frac{\alpha}{2}\right) \frac{\partial^\alpha \omega(x_n, t_m)}{\partial t^\alpha} + \mathcal{O}(k^2) \\ &= \left(\frac{\alpha}{2}\right) \frac{\partial^2 \omega(x_n, t_{m-1})}{\partial x^2} + \left(1 - \frac{\alpha}{2}\right) \frac{\partial^2 \omega(x_n, t_m)}{\partial x^2} \\ &\quad + \left(\frac{\alpha}{2}\right) I_n^{m-1} + \left(1 - \frac{\alpha}{2}\right) I_n^m + \mathcal{O}(k^2).\end{aligned}$$

Approximating the second-order derivatives  $u_{xx}(x_n, t_{m-1})$  and  $u_{xx}(x_n, t_m)$  with the central difference schemes gives

$$\begin{aligned}\frac{1}{k^2} \sum_{s=0}^m \varphi_s^{(\alpha)} + \mathcal{O}(k^2 + h^2) &= \left(1 - \frac{\alpha}{2}\right) \frac{\omega_{n-1}^m - 2\omega_n^m + \omega_{n+1}^m}{h^2} \\ &\quad + \left(\frac{\alpha}{2}\right) \frac{\omega_{n-1}^{m-1} - 2\omega_n^{m-1} + \omega_{n+1}^{m-1}}{h^2} \\ &\quad + \left(\frac{\alpha}{2}\right) I_n^{m-1} + \left(1 - \frac{\alpha}{2}\right) I_n^m.\end{aligned}$$

If  $\zeta = \frac{k^2}{h^2}$ , then the solution of (2.6.14) satisfies

$$\begin{aligned}\omega_n^m - \left(1 - \frac{\alpha}{2}\right) \zeta (\omega_{n-1}^m - 2\omega_n^m + \omega_{n+1}^m) + k^\alpha \mathcal{O}(k^2 + h^2) &= - \sum_{s=2}^m \varphi_s^{(\alpha)} \omega_n^{m-k} + \alpha \omega_n^{m-1} \\ &\quad + \frac{\alpha \zeta}{2} (\omega_{n-1}^{m-1} - 2\omega_n^{m-1} + \omega_{n+1}^{m-1}) + k^\alpha \left[ \left(\frac{\alpha}{2}\right) I_n^{m-1} + \left(1 - \frac{\alpha}{2}\right) I_n^m \right].\end{aligned}\quad (2.6.16)$$

Let  $\mathbf{x} = (x_n)$  be an  $N - 1$ -dimensional vector, the maximum norm infinity of the vector  $\mathbf{x}$  is computed as

$$\|\mathbf{x}\| = \max_{1 \leq n \leq N-1} |x_n|.$$

The vectors  $B_m$ ,  $I_m$  and  $S_m$  are defined as

$B_m = (\omega_n^m)_{n=1}^{N-1}$ , denotes a vector of values of the exact solution at time  $t = mk$ ;

$I_m = \left[ \left(\frac{\alpha}{2}\right) I_n^{m-1} + \left(1 - \frac{\alpha}{2}\right) I_n^m \right]_{n=1}^{N-1}$ ;

$S_m = (s_n^m)_{n=1}^{N-1}$ , represents a vector of the truncation errors at time  $t = mk$ .

It has been shown in (2.6.16) that  $\|S^m\| \in \mathcal{O}(k^\alpha(k^2 + h^2))$ . The entries of the vector  $S_m$  satisfies

$$|s_n^m| < S k^\alpha(k^2 + h^2),$$

where  $S > 1$  is a constant.

Let  $\psi_n^{(\alpha)} = -\varphi_n^{(\alpha)}$  and  $\mathbf{L} = L_{N-1}$  be a tridiagonal matrix obtained from second-order central difference operator [26–30]

$$\mathbf{L} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \quad \text{and} \quad \mathbf{M} = \begin{pmatrix} m_2 & m_1 & & & \\ m_3 & m_2 & m_1 & & \\ & m_3 & m_2 & m_1 & \\ & & m_3 & m_2 & m_1 \\ & & & m_3 & m_2 \end{pmatrix}. \quad (2.6.17)$$

The numbers  $\psi_n^{(\alpha)}$  are positive for  $n \geq 1$  and  $\sum_{n=1}^{\infty} \psi_n^{(\alpha)} = 1$ . We determine the eigenvalues of tridiagonal matrix  $\mathbf{L}$  from the general result for eigenvalues given by [5]

$$\Lambda_l = m_2 + 2m_1 \sqrt{\frac{m_3}{m_1}} \cos\left(\frac{\pi l}{N}\right), \quad l = 1, 2, 3, \dots, N-1. \quad (2.6.18)$$

**Lemma 2.6.3** *The eigenvalues of the tridiagonal matrix  $\mathbf{M} = M_{N-1}$  with elements  $m_2$  on the main diagonal and respective entries  $m_1$  and  $m_3$  on the first diagonals below and above the main diagonal are given by (2.6.18).*

**Corollary 2.6.4** *The matrix  $\mathbf{L}$  has eigenvalues*

$$\Lambda_l = 4 \sin^2\left(\frac{\pi l}{N}\right), \quad l = 1, 2, 3, \dots, N-1.$$

*Proof* With  $m_1 = m_3 = -1$  and  $m_2 = 2$ , we have

$$\Lambda_l = 2 - 2 \cos\left(\frac{\pi l}{N}\right) = 4 \sin^2\left(\frac{\pi l}{N}\right).$$

□

In a matrix form, Eq.(2.6.16) can be written as

$$\left(\mathbf{I} + \left(1 - \frac{\alpha}{2}\right)\zeta\mathbf{L}\right) B_m = \left(\alpha\mathbf{I} - \frac{\alpha}{2}\zeta\mathbf{L}\right) B_{m-1} + \sum_{s=2}^{m-1} \psi_s^{(\alpha)} B_{m-s} + k^\alpha I_m + S_m.$$

Let  $\mathbf{X}$  and  $\mathbf{Y}$  be the matrices

$$\mathbf{X} = \mathbf{I} + \left(\alpha\mathbf{I} - \frac{\alpha}{2}\right)\zeta\mathbf{L} \quad \text{and} \quad \mathbf{Y} = \mathbf{I} - \frac{\zeta}{2}\mathbf{L}.$$

Then

$$\mathbf{X}B_m = \alpha\mathbf{Y}B_{m-1} + \sum_{s=2}^{m-1} \psi_s^{(\alpha)} B_{m-s} + k^\alpha I_m + S_m.$$

We compute an approximation  $\tilde{B}_m$  to the exact solution  $B_m$  of Eq.(2.6.14) at time  $t_m = mk$  on the grid

$$\{(x_n, t_m) | 1 \leq n \leq N, 1 \leq m \leq M\}$$

with  $\tilde{B}_0 = 0$  and the linear systems

$$\mathbf{X}\tilde{B}_m = \alpha\mathbf{Y}B_{m-1} + \sum_{s=2}^{m-1} \psi_s^{(\alpha)} \tilde{B}_{m-s} + k^\alpha I_m. \tag{2.6.19}$$

The values of the entries of the vector  $I_m$  hold for

$$\left(\frac{\alpha}{2}\right) I_n^{m-1} + \left(1 - \frac{\alpha}{2}\right) I_n^m = I_n^{m-\alpha/2} + \mathcal{O}(k^2).$$

An alternative difference approximation for (2.6.14) is recursively computed with the linear systems as

$$\mathbf{X}\tilde{B}_m = \alpha\mathbf{Y}B_{m-1} + \sum_{s=2}^{m-1} \psi_s^{(\alpha)} \tilde{B}_{m-s} + k^\alpha \bar{I}_m, \tag{2.6.20}$$

where  $\bar{I}_m = \left(I_n^{m-\alpha/2}\right)_{n=1}^{N-1}$ . It has been shown in Theorem 29 of [4] that the implicit difference approximations (2.6.19) and (2.6.20) are unconditionally stable and possess second-order accuracy w.r.t. the space and time variables.

## References

1. H. Bahouri, J.Y. Chemin, R. Danchin, *Fourier Analysis and Nonlinear Partial Differential Equations* (Springer, Berlin, 2011)
2. Z. Cinkir, A fast elementary algorithm for computing the determinant of Toeplitz matrices. *J. Comput. Appl. Math.* **255**, 353–361 (2014)
3. R. Courant, K. Friedrichs, H. Lewy, On partial difference equations of mathematical physics. *IBM J. Res. Dev.* **11**, 215–234 (1967)
4. Y. Dimitrov, Numerical approximations for fractional differential equations. *J. Fract. Calc. Appl.* **5**, 1–45 (2014)
5. H. Ding, C. Li, Numerical algorithms for the fractional diffusion-wave equation with reaction term. *Abstr. Appl. Anal.* Article ID **493406**, 15 (2013)
6. M. El-Mikkawy, A fast algorithm for evaluating  $n$ -th order tri-diagonal determinants. *J. Comput. Appl. Math.* **166**, 581–584 (2004)
7. S.O. Fatunla, *Numerical Methods for IVPs in Ordinary Differential Equations* (Academic Press Inc., Harcourt Brace Jovanovich Publishers, New York, 1988)
8. B. Fornberg, *A Practical Guide to Pseudospectral Methods* (Cambridge University Press, Cambridge, 1996)
9. B. Fornberg, Finite difference method. *Scholarpedia* **6**(10), 9685 (2011)

10. B. Fornberg, T.A. Driscoll, A fast spectral algorithm for nonlinear wave equations with linear dispersion. *J. Comput. Phys.* **155**, 456–467 (1999)
11. G. Gao, Z. Sun, Y. Zhang, A finite difference scheme for fractional sub-diffusion equations on an unbounded domain using artificial boundary conditions. *J. Comput. Phys.* **231**, 2865–2879 (2012)
12. S.D. Gedney, *Introduction to the Finite-Difference Time-Domain (FDTD)-Method for Electromagnetics* (Morgan and Claypool Publishers, Arizona, 2011)
13. S. Hamdi, W.E. Schiesser, G.W. Griffiths, Method of lines. *Scholarpedia* **2**(7), 2859 (2010)
14. J.D. Hoffman, *Numerical Methods for Engineers and Scientists* (Marcel Dekker Inc., New York, 2001)
15. H. Holden, K.H. Karlsen, *Nonlinear Partial Differential Equations, The Abel Symposium* (Springer, Berlin, 2012)
16. R.K. Jain, *Numerical Solution of Differential Equations*, 2nd edn. (Wiley Eastern Limited, New Delhi, 1984)
17. A.A. Kilbas, H.M. Srivastava, J.J. Trujillo, *Theory and Applications of Fractional Differential Equations* (Elsevier, Netherlands, 2006)
18. E. Kilic, M. El-Milkkawy, A computational algorithm for special  $n$ th-order pentadiagonal Toeplitz determinants. *Appl. Math. Comput.* **199**, 820–822 (2008)
19. N. Kreiss, J. Lorenz, *Initial-Boundary Value Problems and the Navier-Stokes Equations* (Academic Press, San Diego, 1989)
20. J.D. Lambert, A. Watson, Symmetric multistep method for periodic initial value problem. *J. Inst. Math. Appl.* **18**, 189–202 (1976)
21. P.D. Lax, R.D. Richtmyer, Survey of the instability of linear finite difference equations. *Commun Pure Appl Math* **9**, 267–293 (1956)
22. P.D. Lax, B. Wendroff, Difference schemes for hyperbolic equations with high order of accuracy. *Commun. Pure Appl. Math.* **17**, 381–398 (1964)
23. R.J. Leveque, *Finite Difference Methods for Ordinary and Partial Differential Equations* (SIAM, Philadelphia, 2007)
24. M.M. Meerschaert, C. Tadjeran, Finite difference approximations for fractional advection-dispersion equations. *J. Comput. Appl. Math.* **172**, 65–77 (2004)
25. G.H. Meyer, *Initial Value Methods for Boundary Value Problems-Theory and Application of Invariant Imbedding* (Academic Press, New York, 1973)
26. K.M. Owolabi, Robust IMEX schemes for solving two-dimensional reaction-diffusion models. *Int. J. Nonlinear Sci. Numer. Simul.* **16**, 271–284 (2015). <https://doi.org/10.1515/ijnsns-2015-0004>
27. K.M. Owolabi, K.C. Patidar, Existence and permanence in a diffusive KiSS model with robust numerical simulations. *Int. J. Differ. Equ.* **2015**(485860), 8 (2015). <https://doi.org/10.1155/2015/485860>
28. K.M. Owolabi, K.C. Patidar, Numerical simulations of multicomponent ecological models with adaptive methods. *Theor. Biol. Med. Model.* **13**, 1 (2016). <https://doi.org/10.1186/s12976-016-0027-4>
29. K.M. Owolabi, K.C. Patidar, Numerical solution of singular patterns in one-dimensional Gray-Scott-like models. *Int. J. Nonlinear Sci. Numer. Simul.* **15**, 437–462 (2014). <https://doi.org/10.1515/ijnsns-2013-0124>
30. K.M. Owolabi, K.C. Patidar, Higher-order time-stepping methods for time-dependent reaction-diffusion equations arising in biology. *Appl. Math. Comput.* **240**, 30–50 (2014)
31. I. Podlubny, *Fractional Differential Equations* (Academic Press, San Diego, 1999)
32. D.L. Powers, *Boundary value Problems and Partial Differential equations* (Elsevier Academic Press, USA, 2006)
33. A.R. Mitchell, D.F. Griffiths, *The Finite Difference Method in Partial Differential Equations* (John Wiley and Sons Ltd, 1980)
34. S. Samko, A. Kilbas, O. Marichev, *Fractional Integrals and derivatives: Theory and Applications* (Gordon and Breach, Amsterdam, 1993)

35. W.E. Schisser, G.W. Griffiths, *A Compendium of Partial Differential Equation Models: Method of Lines Analysis with Matlab* (Cambridge University Press, Cambridge, 2009)
36. T. Sogabe, A fast numerical algorithm for the determinant of a pentadiagonal matrix. *Appl. Math. Comput.* **196**, 835–841 (2008)
37. T. Sogabe, A note on a fast numerical algorithm for the determinant of a pentadiagonal matrix. *Appl. Math. Comput.* **201**, 561–564 (2008)
38. E. Sousa, The controversial stability analysis. *Appl. Math. Comput.* **145**, 777–794 (2003)
39. E. Sousa, Finite difference approximations for a fractional advection diffusion problem. *J. Comput. Phys.* **228**, 4038–4054 (2009)
40. J.C. Strikwerda, *Partial Difference Schemes and Partial Differential Equations* (SIAM, Philadelphia, 2004)
41. J.W. Thomas, *Numerical Partial Differential Equations-Finite Difference Methods* (Springer, New York, 1995)
42. J.W. Thomas, *Numerical Partial Differential Equations: Conservation Laws and Elliptic Equations* (Springer, New York, 1999)
43. L.N. Trefethen, *Finite Difference and Spectral Methods for Ordinary and Partial Differential Equations* (Cornell University, Ithaca, 1996)
44. L.N. Trefethen, *Spectral Methods in MATLAB* (SIAM, Philadelphia, 2000)
45. L.N. Trefethen, M. Embere, *Spectra and Pseudospectra: The Behavior of Nonnormal Matrices and Operators* (Princeton University Press, New Jersey, 2005)

# Chapter 3

## Numerical Approximation of Riemann–Liouville Differentiation



The Riemann–Liouville fractional differential operator has been greatly applied in several fields of science, technology and engineering. However, we have realized from already published materials that some researchers used this operator in their model but employ the approximate numerical representation of the Caputo differential operator to get simulation and study the stability analysis. We therefore aim in this chapter to suggest novel numerical approximation of these fractional differential operators. We shall recall from the definition of these derivatives that they are considered as derivative of convolution; therefore, their numerical representation can be accomplished following the steps of already published and established numerical scheme if one considers the convolution part as e function. In this chapter, we present the numerical representation from Riemann to Caputo–Fabrizio type.

### 3.1 Numerical Approximation for Time Derivative

The step of discretization presented here is similar to the ones reported in earlier works [1, 2]. We shall present directly the numerical approximation; by definition, we have

$$\begin{aligned} U(t) &= \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\tau)^{-\alpha} f(\tau) d\tau, \\ {}_0^{RL} \mathcal{D}_t^\alpha \{f(t)\} &= \frac{d}{dt} U(t), \\ \frac{d}{dt} U(t) &= \frac{U(t_{j+1}) - U(t_j)}{\Delta t}, \end{aligned} \tag{3.1.1}$$

$$U(t_{j+1}) = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{j+1}} (t_{j+1} - \tau)^{-\alpha} f(\tau) d\tau,$$

$$U(t_j) = \frac{1}{\Gamma(1-\alpha)} \int_0^{t_j} (t_j - \tau)^{-\alpha} f(\tau) d\tau.$$

Without loss of generality, we present the numerical approximation as follows:

$$\begin{aligned} U(t_{j+1}) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{j+1}} (t_{j+1} - \tau)^{-\alpha} f(\tau) d\tau, \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} (t_{j+1} - \tau)^{-\alpha} \frac{f(t_{s+1}) + f(t_s)}{2} d\tau, \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^j \frac{f(t_{s+1}) + f(t_s)}{2} \int_{t_s}^{t_{s+1}} (t_{j+1} - \tau)^{-\alpha} d\tau, \\ &= \frac{1}{\Gamma(2-\alpha)} \sum_{s=0}^j \frac{f(t_{s+1}) + f(t_s)}{2} [(t_{j+1} - t_{s+1})^{1-\alpha} - (t_{j+1} - t_s)^{1-\alpha}], \end{aligned} \tag{3.1.2}$$

similarly,

$$\begin{aligned} U(t_j) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_j} (t_j - \tau)^{-\alpha} f(\tau) d\tau, \\ &= \frac{1}{\Gamma(2-\alpha)} \sum_{s=1}^j \frac{f(t_s) + f(t_{s-1})}{2} [(t_j - t_{s-1})^{1-\alpha} - (t_j - t_s)^{1-\alpha}] + \mathcal{O}(\Delta t). \end{aligned} \tag{3.1.3}$$

Thus

$$\begin{aligned} \frac{d}{dt} U(t) &= \frac{1}{\Delta t \Gamma(2-\alpha)} \left[ \sum_{s=0}^j \frac{f(t_{s+1}) + f(t_s)}{2} [(t_{j+1} - t_{s+1})^{1-\alpha} - (t_{j+1} - t_s)^{1-\alpha}] \right. \\ &\quad \left. - \sum_{s=1}^j \frac{f(t_s) + f(t_{s-1})}{2} [(t_j - t_{s-1})^{1-\alpha} - (t_j - t_s)^{1-\alpha}] \right] \\ &\quad + R_{\alpha,j}, \end{aligned} \tag{3.1.4}$$

where

$$R_{\alpha,j} = \frac{1}{\Delta t \Gamma(1-\alpha)} \left\{ \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \frac{f(u) - f(t_{s+1})}{(t_{j+1} - u)^\alpha} du - \sum_{s=0}^{j-1} \int_{t_s}^{t_{s+1}} \frac{f(u) - f(t_{s+1})}{(t_j - u)^\alpha} du \right\}.$$

**Theorem 3.1.1** *Let  $f$  denote a function not necessarily differentiable on  $[a, T]$ ; then the fractional derivative of  $f$  of order  $\alpha$  in the Riemann–Liouville sense is defined by*

$$\begin{aligned} {}_0^{RL}\mathcal{D}_t^\alpha\{f(t)\} &= \frac{1}{\Delta t\Gamma(2-\alpha)} \left[ \sum_{s=0}^j \frac{f(t_{s+1})+f(t_s)}{2} [(t_{j+1}-t_{s+1})^{1-\alpha} - (t_{j+1}-t_s)^{1-\alpha}] \right. \\ &\quad \left. - \sum_{s=1}^j \frac{f(t_s)+f(t_{s-1})}{2} [(t_j-t_{s-1})^{1-\alpha} - (t_j-t_s)^{1-\alpha}] \right] \\ &\quad + R_{\alpha,j}, \end{aligned} \quad (3.1.5)$$

where

$$|R_{\alpha,j}| \leq C \left( t_{j+1}^{1-\alpha} - t_j^{1-\alpha} \right).$$

*Proof* From the formula of  $|R_{\alpha,j}|$  above, we obtain the following:

$$\begin{aligned} \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \frac{f(u) - f(t_{s+1})}{(t_{j+1}-u)^\alpha} du &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \frac{(f(u) - f(t_{s+1}))(u - t_{s+1})}{(u - t_{s+1})(t_{j+1}-u)^\alpha} du \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \frac{(f^{(\prime)}(\lambda_s)(u - t_{s+1}))}{(t_{j+1}-u)^\alpha} du, \quad u < t \leq t_{j+1}. \end{aligned} \quad (3.1.6)$$

Thus,

$$\begin{aligned} &\left| \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \frac{(f^{(\prime)}(\lambda_s)(u - t_{s+1}))}{(t_{j+1}-u)^\alpha} du \right| \leq \\ &\frac{t_{j+1}^{1-\alpha}}{\Gamma(1-\alpha)} \max_{0 \leq t \leq t_{j+1}} |f^{(\prime)}(t)| \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \frac{1}{(i_{j+1}-u)^\alpha} du \leq \frac{\Delta t}{\Gamma(2-\alpha)} \max_{0 \leq t \leq t_{j+1}} |f^{(\prime)}(t)| t_{j+1}^{1-\alpha}. \end{aligned} \quad (3.1.7)$$

Also,

$$\left| \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^{j-1} \int_{t_s}^{t_{s+1}} \frac{(f(u) - f(t_{s+1}))}{(t_j - u)^\alpha} du \right| \leq \frac{\Delta t}{\Gamma(2-\alpha)} \max_{0 \leq t \leq t_{j+1}} |f^{(\prime)}(t)| t_j^{1-\alpha}.$$

The required result is thus obtained with

$$C = \frac{1}{\Gamma(2-\alpha)} \max_{0 \leq t \leq t_{j+1}} |f^{(\prime)}(t)|.$$

□

### 3.2 Numerical Approximation for Space First-Order Derivative

By definition, the first-order partial derivative in space is given by

$$\left(\frac{\partial u(x, t)}{\partial x}\right)_i \approx \frac{u_{i+1}^j - u_i^j}{\Delta x} \quad (\text{forward difference}), \quad (3.2.1)$$

$$\approx \frac{u_i^j - u_{i-1}^j}{\Delta x} \quad (\text{backward difference}), \quad (3.2.2)$$

$$\approx \frac{u_{i+1}^j - u_{i-1}^j}{\Delta x} \quad (\text{central difference}) \quad (3.2.3)$$

and

$$\left(\frac{\partial u(x, t)}{\partial x}\right)_i \approx \frac{1}{2} \left( \frac{f_{i+1}^{j+1} - f_i^{j+1}}{2(\Delta x)} + \frac{f_i^j - C_{i-1}^j}{2(\Delta x)} \right), \quad (\text{Crank–Nicholson scheme}). \quad (3.2.4)$$

Recall,

$$\begin{aligned} {}_0^{RL}\mathcal{D}_x^\alpha f(x, t) &= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^x (x-\tau)^{-\alpha} f(\tau, t) d\tau \\ &= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} F(x, t). \end{aligned} \quad (3.2.5)$$

By forward difference scheme, we have

$${}_0^{RL}\mathcal{D}_x^\alpha f(x_i, t_j) \simeq \frac{1}{\Gamma(1-\alpha)} \frac{F_{i+1}^j - F_i^j}{\Delta x}, \quad (3.2.6)$$

where

$$\begin{aligned} F_{i+1}^j &= \int_0^{x_{i+1}} (x_{i+1} - \tau)^{-\alpha} f(\tau, t_j) d\tau \\ &= \sum_{k=0}^i \int_{x_k}^{x_{k+1}} (x_{i+1} - \tau)^{-\alpha} f(x_k, t_j) d\tau \\ &= \sum_{k=0}^i f(x_k, t_j) \int_{x_k}^{x_{k+1}} (x_{i+1} - \tau)^{-\alpha} d\tau. \end{aligned} \quad (3.2.7)$$

We let  $x_{i+1} = y$ , so that  $dy = -d\tau$ , which implies  $-dy = d\tau$ ,  $y = x_{k+1} - x_k$  and  $y = x_{i+1} - x_{k+1}$ , then

$$\begin{aligned}
F_{i+1}^j &= \sum_{k=0}^i f(x_k, t_j) \int_{x_{i+1}-x_{k+1}}^{x_{i+1}-x_k} y^{-\alpha} dy \\
&= \sum_{k=0}^i f(x_k, t_j) \frac{y^{1-\alpha}}{1-\alpha} \Big|_{x_{i+1}-x_{k+1}}^{x_{i+1}-x_k} \\
&= \sum_{k=0}^i \frac{f(x_k, t_j)}{1-\alpha} \left\{ (x_{i+1}-x_k)^{1-\alpha} - (x_{i+1}-x_{k+1})^{1-\alpha} \right\}.
\end{aligned}$$

With substitution  $x_{i+1} = (i+1)\Delta x$ ,  $x_k = k\Delta$ , this implies that  $x_{i+1} - x_k = x_{i+1} - x_k = (i+1-k)\Delta x$  and  $x_{i+1} - x_{k+1} = x_{i+1} - x_k = (i+2-k)\Delta x$ , we obtain

$$F_{i+1}^j = \sum_{k=0}^i \frac{f(x_k, t_j)}{1-\alpha} (\Delta x)^{1-\alpha} \left\{ (i+1-k)^{1-\alpha} - (i-k)^{1-\alpha} \right\}. \quad (3.2.8)$$

Similarly,

$$\begin{aligned}
F_i^j &= \int_0^{x_i} (x_i - \tau)^{-\alpha} f(\tau, t_j) d\tau \\
&= \sum_{k=0}^i \int_{x_k}^{x_{k+1}} (x_{i+1} - \tau)^{-\alpha} f(x_k, t_j) d\tau \\
&= \sum_{k=0}^{i-1} f(x_k, t_j) \int_{x_k}^{x_{k+1}} (x_i - \tau)^{-\alpha} d\tau.
\end{aligned} \quad (3.2.9)$$

We let  $x_i = y$ , so that  $dy = -d\tau$ , which implies  $-dy = d\tau$ ,  $y = x_{k+1} - x_k$  and  $y = x_i - x_{k+1}$ , then

$$\begin{aligned}
F_i^j &= \sum_{k=0}^i f(x_k, t_j) \int_{x_i-x_{k+1}}^{x_i-x_k} y^{-\alpha} dy \\
&= \sum_{k=0}^i f(x_k, t_j) \frac{y^{1-\alpha}}{1-\alpha} \Big|_{x_i-x_{k+1}}^{x_i-x_k} \\
&= \sum_{k=0}^{i-1} \frac{f(x_k, t_j)}{1-\alpha} \left\{ (x_i - x_k)^{1-\alpha} - (x_i - x_{k+1})^{1-\alpha} \right\}.
\end{aligned}$$

With substitution  $x_i = (i)\Delta x$ ,  $x_k = k\Delta$ , this implies that  $x_i - x_k = x_i - x_k = (i-k)\Delta x$  and  $x_i - x_{k+1} = x_i - x_k = (i-k-1)\Delta x$ , we obtain

$$F_i^j = \sum_{k=0}^{i-1} \frac{f(x_k, t_j)}{1-\alpha} (\Delta x)^{1-\alpha} \left\{ (i-k)^{1-\alpha} - (i-k-1)^{1-\alpha} \right\}. \quad (3.2.10)$$

With backward–forward difference scheme, we obtain the following approximation. We define the Riemann–Liouville derivative as

$$\begin{aligned} {}_0^{RL}\mathcal{D}_x^\alpha f(x, t) &= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} \int_0^x (x-y)^{-\alpha} f(y, t) dy \\ &= \frac{1}{\Gamma(1-\alpha)} \frac{d}{dx} G(x, t). \end{aligned} \quad (3.2.11)$$

$${}_0^{RL}\mathcal{D}_x^\alpha f(x_i, t_j) = \frac{1}{\Gamma(1-\alpha)} \frac{G_i^j - G_{i-1}^j}{\Delta x},$$

where

$$\begin{aligned} G_i^j &= \int_0^{x_i} (x_i - y)^{-\alpha} f(y, t_j) dy \\ &= \sum_{k=0}^{i-1} \int_{x_k}^{x_{k+1}} (x_i - y)^{-\alpha} f(x_k, t_j) dy \\ &= \sum_{k=0}^{i-1} f(x_{i-1}, t_j) \int_{x_k}^{x_{k+1}} (x_i - y)^{-\alpha} dy \\ &= \sum_{k=0}^{i-1} f(x_{i-1}, t_j) \int_{x_i - x_{k+1}}^{x_i - x_k} y^{-\alpha} dy \\ &= \sum_{k=0}^{i-1} f(x_{i-1}, t_j) \frac{(\Delta x)^{1-\alpha}}{1-\alpha} [(i-k)^{1-\alpha} - (i-1-k)^{1-\alpha}] \end{aligned} \quad (3.2.12)$$

and

$$\begin{aligned} G_{i-1}^j &= \int_0^{x_{i-1}} (x_{i-1} - y)^{-\alpha} f(y, t_j) dy \\ &= \sum_{k=0}^{i-2} \int_{x_k}^{x_{k+1}} (x_{i-1} - y)^{-\alpha} f(x_k, t_j) dy \\ &= \sum_{k=0}^{i-2} f(x_{i-2}, t_j) \int_{x_k}^{x_{k+1}} (x_{i-1} - y)^{-\alpha} dy \\ &= \sum_{k=0}^{i-2} f(x_{i-2}, t_j) \int_{x_{i-1} - x_{k+1}}^{x_{i-1} - x_k} y^{-\alpha} dy \\ &= \sum_{k=0}^{i-2} f(x_{i-2}, t_j) \frac{(\Delta x)^{1-\alpha}}{1-\alpha} [(i-1-k)^{1-\alpha} - (i-2-k)^{1-\alpha}]. \end{aligned} \quad (3.2.13)$$

### 3.3 Numerical Approximation for Space Second-Order Derivative

The space second-order approximation that we present in this section follows the discretization approach as in some earlier works [3–5]. We present directly the discretization scheme, and from the definition of fractional derivative of order less or equal to two and greater than 1, we have

$$U(x) = \frac{1}{\Gamma(2-\alpha)} \int_0^x (x-\tau)^{\alpha-2} f(\tau) d\tau,$$

and

$${}^RL\mathcal{D}_t^\alpha\{f(x)\} = \frac{d^2U(x)}{dx^2}.$$

By using the numerical approximation of the second derivative, we have

$${}^RL\mathcal{D}_t^\alpha\{f(x)\} = \frac{d^2U(x)}{dx^2} = \frac{U(x_{i+1}) - 2U(x_i) + U(x_{i-1}))}{2(\Delta x)^2}, \quad (3.3.1)$$

so that

$$\begin{aligned} U(x_{i+1}) &= \frac{1}{\Gamma(2-\alpha)} \int_0^{x_{i+1}} (x_{i+1}-\nu)^{1-\alpha} f(\nu) d\nu, \\ &= \frac{1}{\Gamma(2-\alpha)} \sum_{s=0}^j \int_{x_s}^{x_{s+1}} (x_{i+1}-\nu)^{1-\alpha} f(x_{s+1}) d\nu + E_1, \\ &= \frac{1}{\Gamma(2-\alpha)} \sum_{s=0}^j f(x_{s+1}) \int_{x_s}^{x_{s+1}} (x_{i+1}-\nu)^{1-\alpha} d\nu + E_1, \\ &= \frac{1}{\Gamma(3-\alpha)} \sum_{s=0}^j f(x_{s+1}) \left\{ (x_{i+1}-x_{s+1})^{1-\alpha} - (x_{i+1}-x_s)^{1-\alpha} \right\} + E_1, \quad (3.3.2) \\ &= \frac{(\Delta)^{1-\alpha}}{\Gamma(3-\alpha)} \sum_{s=0}^j f(x_{s+1}) \left\{ (j-s)^{1-\alpha} - (j-s+1)^{1-\alpha} \right\} + E_1, \\ &= \frac{(\Delta)^{1-\alpha}}{\Gamma(3-\alpha)} \sum_{s=0}^j f(x_{s+1}) \bar{h}_{j,s}^\alpha + E_1, \end{aligned}$$

where

$$\begin{aligned} E_1 &= \frac{1}{\Gamma(2-\alpha)} \sum_{s=0}^j f(x_{s+1}) \int_{x_s}^{x_{s+1}} \frac{f(\nu) - f(x_{s+1})}{(x_{s+1}-\nu)^{\alpha-1}} d\nu \quad (3.3.3) \\ \bar{h}_{j,s}^\alpha &= (j-s)^{1-\alpha} - (j-s+1)^{1-\alpha}. \end{aligned}$$

Also, with the same approach, we equally obtain

$$\begin{aligned}
 U(x_j) &= \frac{(\Delta)^{1-\alpha}}{\Gamma(3-\alpha)} \sum_{s=0}^{j-1} f(x_{s+1}) \hbar_{j,s}^\alpha + E_2, \\
 E_2 &= \frac{1}{\Gamma(2-\alpha)} \sum_{s=0}^{j-1} \int_{x_s}^{x_{s+1}} \frac{f(\nu) - f(x_{s+1})}{(x_{s+1} - \nu)^{\alpha-1}} d\nu \hbar_{j,s}^\alpha = (j-s)^{1-\alpha} - (j-s+1)^{1-\alpha},
 \end{aligned} \tag{3.3.4}$$

$$\begin{aligned}
 U(x_{j-1}) &= \frac{(\Delta)^{1-\alpha}}{\Gamma(3-\alpha)} \sum_{s=1}^{j-1} f(x_{s+1}) \hbar_{j,s}^{\alpha,2} + E_3, \\
 E_3 &= \frac{1}{\Gamma(2-\alpha)} \sum_{s=0}^{j-1} \int_{x_s}^{x_{s+1}} \frac{f(\nu) - f(x_{s+1})}{(x_{s+1} - \nu)^{\alpha-1}} d\nu \hbar_{j,s}^{\alpha,2} = (j-s-2)^{1-\alpha} - (j-s+1)^{1-\alpha}.
 \end{aligned}$$

Substituting Eqs. (3.3.3) and (3.3.4) in Eq. (3.3.1), we get

$${}^{RL}\mathcal{D}_t^\alpha \{f(x)\} = \frac{(\Delta x)^{-1-\alpha}}{2\Gamma(3-\alpha)} \left[ \sum_{s=0}^j f(x_{s+1}) \hbar_{j,s}^\alpha - \sum_{s=0}^{j-1} f(x_{s+1}) \hbar_{j,s}^{\alpha,1} + \sum_{s=0}^{j-1} f(x_{s+1}) \hbar_{j,s}^{\alpha,2} \right] + E_{\alpha,j,s}, \tag{3.3.5}$$

where

$$\begin{aligned}
 E_{\alpha,j,s} &= \frac{(\Delta x)^{-2}}{2\Gamma(2-\alpha)} \left[ \sum_{s=0}^j \int_{x_s}^{x_{s+1}} \frac{f(\nu) - f(x_{s+1})}{(x_{j+1} - \nu)^{\alpha-1}} d\nu - 2 \sum_{s=0}^{j-1} \int_{x_s}^{x_{s+1}} \frac{f(\nu) - f(x_{s+1})}{(x_j - \nu)^{\alpha-1}} d\nu \right. \\
 &\quad \left. + \sum_{s=1}^{j-1} \int_{x_s}^{x_{s+1}} \frac{f(\nu) - f(x_{s+1})}{(x_{j-1} - \nu)^{\alpha-1}} d\nu \right],
 \end{aligned} \tag{3.3.6}$$

and

$$\begin{aligned}
 \hbar_{j,s}^\alpha &= (j-s)^{1-\alpha} - (j-s+1)^{1-\alpha}, \\
 \hbar_{j,s}^{\alpha,1} &= (j-s-1)^{1-\alpha} - (j-s)^{1-\alpha}, \\
 \hbar_{j,s}^{\alpha,2} &= (j-s-2)^{1-\alpha} - (j-s-1)^{1-\alpha}.
 \end{aligned} \tag{3.3.7}$$

Without loss of generality, we evaluate

$$\begin{aligned}
 |E_1| &= \left| \frac{1}{\Gamma(2-\alpha)} \sum_{s=0}^{x_{s+1}} \frac{f(\nu) - f(x_{s+1})}{(x_{j+1} - \nu)^{\alpha-1}} d\nu \right|, \\
 &= \left| \frac{1}{\Gamma(2-\alpha)} \sum_{s=0}^j \int_{x_s}^{x_{s+1}} \frac{f'(\lambda_k)(\nu - x_{s+1})}{(x_{j+1} - \nu)^{\alpha-1}} d\nu \right| \quad \nu < \lambda_s < x_{j+1}, \tag{3.3.8} \\
 &\leq \frac{\Delta x}{\Gamma(2-\alpha)} \max_{0 \leq x \leq x_{j+1}} |f'(x)| \sum_{s=0}^j \int_{x_s}^{x_{s+1}} \frac{1}{(x_{j+1} - \nu)^{\alpha-1}} d\nu,
 \end{aligned}$$

$$\leq \frac{(\Delta x)^{1-\alpha}}{\alpha\Gamma(2-\alpha)} \max_{0 \leq x \leq x_{j+1}} |f'(x)| x_{j+1}^{-\alpha}.$$

Similarly,

$$|E_2| \leq \frac{(\Delta x)^{1-\alpha}}{\alpha\Gamma(2-\alpha)} \max_{0 \leq x \leq x_{j+1}} |f'(x)| x_j^{-\alpha},$$

and

$$|E_3| \leq \frac{(\Delta x)^{1-\alpha}}{\alpha\Gamma(2-\alpha)} \max_{0 \leq x \leq x_{j+1}} |f'(x)| x_{j-1}^{-\alpha}.$$

**Theorem 3.3.1** *Let  $f$  be a function not necessary differentiable on interval  $[a, T]$ ; then, the fractional derivative of  $f$  of order  $1 < \alpha < 2$  in the Riemann–Liouville sense is*

$${}^R\mathcal{D}_t^\alpha\{f(x)\} = \frac{(\Delta x)^{-1-\alpha}}{2\Gamma(3-\alpha)} \left[ \sum_{s=0}^j f(x_{s+1})h_{j,s}^\alpha - 2 \sum_{s=0}^{j-1} f(x_{s+1})h_{j,s}^{\alpha,1} + \sum_{s=0}^{j-1} f(x_{s+1})h_{j,s}^{\alpha,2} \right] + E_{\alpha,j,s},$$

where

$$E_{\alpha,j,s} \leq \frac{(\Delta x)^{-2}}{2\Gamma(2-\alpha)} C_1.$$

*Proof* The proof follows directly from Theorem 3.1.1. □

### 3.4 Crank–Nicholson Scheme for Time-Fractional Differential Equations in Riemann–Liouville Sense

In this section, we propose a Crank–Nicholson scheme with accuracy of order  $\mathcal{O}(k^2 + h^2)$  for time-fractional equations with the Riemann–Liouville derivative. We consider the time-fractional heat or diffusion equation

$$\begin{aligned} \frac{\mathfrak{M}\partial^\alpha u(x,t)}{\partial t^\alpha} &= \frac{\partial^2 u}{\partial x^2} + f(t,x), & 0 < \alpha \leq 1, & \quad 0 < x < 1, \quad 0 < t < 1 \\ u(x,0) &= g(x), & & \quad 0 \leq x \leq 1 \\ u(0,t) &= u(1,t) = 0, & & \quad 0 \leq t \leq 1, \end{aligned} \tag{3.4.1}$$

where the term  $\mathfrak{M}\partial^\alpha u(x,t)/\partial t^\alpha$  represents  $\alpha$ -order modified Riemann–Liouville fractional derivative [6, 7] with the given definition

$$\begin{aligned} \frac{\mathfrak{M}\partial^\alpha u(x, t)}{\partial t^\alpha} &= \frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{u(x, \tau) - u(x, 0)}{(t-\tau)^\alpha} d\tau, \quad \text{for } 0 < \alpha < 1, \\ &= \frac{\partial}{\partial t} u(x, t), \quad \text{for } \alpha = 1, \end{aligned} \quad (3.4.2)$$

where  $\Gamma(\cdot)$  is usual Gamma function.

For the discretization issue, we introduce the basic ideas for the numerical solution of (3.4.1) using the Crank–Nicholson difference scheme. Let  $M$  and  $N$  be some positive integers that represent the grid sizes in space and time for the finite difference scheme define by  $h = 1/M$  and  $k = 1/N$ , respectively. The grid points in the time interval  $[0, 1]$  are  $t_n = nk$ ,  $n = 0, 1, 2, \dots, N$ , and the grid points in the space direction on  $[0, 1]$  are numbers  $x_i = ih$ ,  $i = 0, 1, 2, \dots, M$ . At grid points, the values of functions  $u$  and  $f$  are, respectively, denoted as  $u_i^n = u(x_i, t_n)$  and  $f_i^n = f(x_i, t_n)$ .

To obtain a discrete approximation to the derivative  $\partial^\alpha u(x, t)/\partial t^\alpha$  at  $(x_i, t_{n+\frac{1}{2}})$ , just as in the classical Crank–Nicholson difference case. We let

$$G(x, t) = \frac{1}{\gamma(1-\alpha)} \int_0^t \frac{u(x, \tau) - u(x, 0)}{(t-\tau)^\alpha} d\tau. \quad (3.4.3)$$

Then, we obtain

$$\frac{\partial^\alpha u(x_i, t_{n+\frac{1}{2}})}{\partial t^\alpha} = \frac{\partial}{\partial t} G(x_i, t_{n+\frac{1}{2}}) = \frac{G(x_i, t_{n+1}) - G(x_i, t_n)}{k} + \mathcal{O}(k^2). \quad (3.4.4)$$

Next, we obtain numerical approximations for  $G(x_i, t_{n+1})$  and  $G(x_i, t_n)$  in the form

$$\begin{aligned} G(x_i, t_{n+1}) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{n+1}} \frac{u(x_i, \tau) - u(x_i, 0)}{t_{n+1} - \tau} d\tau \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^{n+1} \int_{(j-1)k}^{jk} \frac{u(x_i, \tau)}{(t_{n+1} - \tau)^\alpha} d\tau - u(x_i, 0) \frac{((n+1)k)^{1-\alpha}}{\Gamma(2-\alpha)} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^{n+1} \int_{(j-1)k}^{jk} \left[ \frac{(\tau - t_j)}{-k} u_i^{j-1} + \frac{(\tau - t_{j-1})}{k} u_i^j + \mathcal{O}(k^2) \right] \frac{1}{(t_{n+1} - \tau)^\alpha} d\tau \\ &\quad - u_i^0 \frac{((n+1)k)^{1-\alpha}}{\Gamma(2-\alpha)} \quad (3.4.5) \\ &= k \sum_{j=0}^n (p_j - jq_j) u_i^{n-j} - k \sum_{j=0}^n (p_j - (j+1)q_j) u_i^{n-j+1} - u_i^0 \frac{((n+1)k)^{1-\alpha}}{\Gamma(2-\alpha)} + T_{n+1}, \end{aligned}$$

where

$$\begin{aligned}
T_{n+1} &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^{n+1} \int_{(j-1)k}^{jk} \mathcal{O}(k^2) \frac{d\tau}{(t_{n+1}-\tau)^\alpha} \\
&= \frac{1}{(1-\alpha)\Gamma(1-\alpha)} \mathcal{O}(k^2) \sum_{j=1}^{n+1} [(n-j+2)^{1-\alpha} - (n-j+1)^{1-\alpha}] k^{1-\alpha} \\
&= \frac{1}{\Gamma(2-\alpha)} (n+1)^{1-\alpha} + \mathcal{O}(k^{3-\alpha}).
\end{aligned}$$

In the same manner, one obtains

$$\begin{aligned}
G(x_i, t_n) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_n} \frac{u(x_i, \tau) - u(x_i, 0)}{(t_n - \tau)^\alpha} d\tau \\
&= k \sum_{j=1}^n (p_{j-1} - (j-1)q_{j-1}) u_i^{n-j} - k \sum_{j=1}^n (p_{j-1} - jq_{j-1}) u_i^{n-j+1} - u_i^0 \frac{(nk)^{1-\alpha}}{\Gamma(2-\alpha)} + T_n,
\end{aligned}$$

where

$$T_n = \frac{1}{\Gamma(2-\alpha)} n^{1-\alpha} \mathcal{O}(k^{3-\alpha}),$$

$$p_j = \frac{k^{-\alpha}}{(2-\alpha)\Gamma(1-\alpha)} [(j+1)^{2-\alpha} - j^{2-\alpha}],$$

and

$$q_j = \frac{k^{-\alpha}}{(1-\alpha)\Gamma(1-\alpha)} [(j+1)^{1-\alpha} - j^{1-\alpha}].$$

Hence, with the above expressions we have the following approximation:

$$\begin{aligned}
\frac{\partial^\alpha u(x_i, t_{n+\frac{1}{2}})}{\partial t^\alpha} &= \frac{G(x_i, t_{n+1}) - G(x_i, t_n)}{k} + \mathcal{O}(k^2) \\
&= b_n u_i^0 + \sum_{j=0}^n a_j u_i^{n+1-j} + \frac{T_{n+1} - T_n}{k} + \mathcal{O}(k^2) \tag{3.4.6} \\
&= b_n u_i^0 + \sum_{j=0}^n a_j u_i^{n+1-j} + \frac{1}{\Gamma(2-\alpha)} [(n+1)^{1-\alpha} - n^{1-\alpha}] \mathcal{O}(k^{2-\alpha}) + \mathcal{O}(k^2) \\
&= b_n u_i^0 + \sum_{j=0}^n a_j u_i^{n+1-j} + \frac{1}{\Gamma(2-\alpha)} \left[ \frac{(n+1)^{1-\alpha} - n^{1-\alpha}}{k} \right] \mathcal{O}(k^{3-\alpha}) + \mathcal{O}(k^2) \\
&= b_n u_i^0 + \sum_{j=0}^n a_j u_i^{n+1-j} + \frac{1}{\Gamma(2-\alpha)} \left[ \frac{(k(n+1))^{1-\alpha} - (kn)^{1-\alpha}}{k} \right] \mathcal{O}(k^2) + \mathcal{O}(k^2),
\end{aligned}$$

where

$$b_0 = 3p_0 - p_1 + 2q_1 - 2q_0$$

$$b_n = p_n - p_{n-1} + (n-1)q_{n-1} - (n+1)q_n, \quad 1 \leq n \leq N-1,$$

$$a_0 = q_0 - p_0,$$

$$a_1 = 2p_0 - p_1 + 2q_1 - q_0,$$

$$a_j = (-p_{j-2} + 2p_{j-1} - p_j) + (j-2)q_{j-2} - (2j-1)q_{j-1} + (j+1)q_j, \quad j \geq 2.$$

By adopting the mean-value theorem technique, one gets

$$\frac{(k(n+1))^{1-\alpha} - (kn)^{1-\alpha}}{k} = f'(e) = \text{a constant},$$

note that  $f(x) = x^{1-\alpha}$  and  $t_n < e < t_{n+1}$ . So, for the modified Riemann–Liouville fractional derivative, we have the following second-order approximation:

$$\begin{aligned} \frac{\partial^\alpha u(x_i, t_{n+\frac{1}{2}})}{\partial t^\alpha} &= \frac{G(x_i, t_{n+1}) - G(x_i, t_n)}{k} + \mathcal{O}(k^2) \\ &= b_n u_i^0 + \sum_{j=0}^n a_j u_i^{n+1-j} + \mathcal{O}(k^2). \end{aligned} \quad (3.4.7)$$

### The Crank–Nicholson Difference Scheme

By using the above approximation, we obtain the second-order accurate Crank–Nicholson difference scheme

$$\begin{aligned} b_n u_i^0 + \sum_{j=0}^n a_j u_i^{n+1-j} - \left( \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{2h^2} + \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{2h^2} \right) \\ = f\left(x_i, t_{n+\frac{k}{2}}\right), \quad 0 \leq n \leq N-1, \quad 1 \leq i \leq M-1, \quad (3.4.8) \\ u_i^0 = \phi(x_i), \quad 1 \leq i \leq M-1, \\ u_0^n = 0, \quad u_M^n = 0, \quad 0 \leq n \leq N. \end{aligned}$$

On rearranging, we have

$$\begin{aligned} \left(-\frac{1}{2h^2}\right)(u_{i+1}^{n+1} + u_{i+1}^n) + b_n u_i^0 + \sum_{j=0}^n a_j u_i^{n+1-j} + \left(-\frac{1}{2h^2}\right)(u_{i+1}^{n+1} + u_{i+1}^n) \\ = f\left(x_i, t_{n+\frac{k}{2}}\right), \quad 0 \leq n \leq N-1, \quad 1 \leq i \leq M-1, \quad (3.4.9) \\ u_i^0 = \phi(x_i), \quad 1 \leq i \leq M-1, \\ u_0^n = 0, \quad u_M^n = 0, \quad 0 \leq n \leq N, \end{aligned}$$

which we transform into matrix



$$\begin{aligned} \mathbf{P} + \mathbf{Q}\mathbf{p}_{i+1} + \mathbf{P}\mathbf{p}_i\mathbf{p}_{i+1} &= 0, \\ \mathbf{Q}\mathbf{q}_{i+1} + \mathbf{P}\mathbf{p}_i\mathbf{q}_{i+1} + \mathbf{P}\mathbf{q}_i &= \nu_i, \quad 1 \leq i \leq M-1. \end{aligned}$$

Finally, we obtain the pair formulas

$$\begin{aligned} \mathbf{p}_{i+1} &= -(\mathbf{Q} + \mathbf{P}\mathbf{p}_i)^{-1}\mathbf{P}, \\ \mathbf{q}_{i+1} &= -(\mathbf{Q} + \mathbf{P}\mathbf{p}_i)^{-1}(\nu_i - \mathbf{P}\mathbf{q}_i), \quad 1 \leq i \leq M-1. \end{aligned} \quad (3.4.15)$$

### Stability of the Scheme

The stability analysis of the method is examined by using the analysis of the eigenvalues of the iteration matrix  $\mathbf{p}_i$  ( $1 \leq i \leq M$ ) of (3.4.13). We let  $\mu(\mathbf{P})$  be the spectral radius of a matrix  $\mathbf{P}$ , i.e. the maximum eigenvalue of  $\mathbf{P}$ .

We want  $\mu(p_i) < 1$  ( $1 \leq i \leq M$ ), by induction. Bear in mind that  $\mathbf{p}_1$  is a zero matrix  $\mu(\mathbf{p}_1) = 0 < 1$ .

Moreover,

$$p_2 = -\mathbf{Q}^{-1}\mathbf{P}, \quad \mu(p_2) = \mu(-\mathbf{Q}^{-1}\mathbf{P}) = \frac{-1}{1/h^2 + a_0} \cdot \frac{-1}{2h^2} = \frac{1}{h^2} \cdot \frac{1}{2(1/h^2 + a_0)},$$

and  $p_2$  takes the form

$$p_2 = \begin{pmatrix} 0 & & & & \\ \frac{1/h^2}{2(1/h^2 + a_0)} & & & & \\ & \frac{1/h^2}{2(1/h^2 + a_0)} & & & \\ & & \ddots & & \\ & & & \frac{1/h^2}{2(1/h^2 + a_0)} & \\ & & & & 0 \end{pmatrix}_{(N+1) \times (N+1)}, \quad (3.4.16)$$

where

$$a_0 = q_0 - p_0 = \frac{k^{-\alpha}}{(1-\alpha)\Gamma(1-\alpha)} - \frac{k^{-\alpha}}{(2-\alpha)\Gamma(1-\alpha)} = \frac{k^{-\alpha}}{\Gamma(3-\alpha)} > 0,$$

therefore, one concludes that  $\mu(p_2) < 1$ .

Again, let us assume that  $\mu(\mathbf{p}_i) < 1$ . After some algebraic manipulations, we have that

$$\begin{aligned} \mathbf{p}_{i+1} &= -(\mathbf{Q} + \mathbf{P}\mathbf{p}_i)^{-1}\mathbf{P} \\ &= \left( \frac{1}{2h^2} \right) \begin{pmatrix} 0 & & & & \\ \frac{1}{\mathbf{Q}_{2,2} - (1/2h^2)\mathbf{p}_{i,2,2}} & & & & \\ & \frac{1}{\mathbf{Q}_{3,3} - (1/2h^2)\mathbf{p}_{i,3,3}} & & & \\ & & \ddots & & \\ & & & \frac{1}{\mathbf{Q}_{N+1,N+1} - (1/2h^2)\mathbf{p}_{i,N+1,N+1}} & \\ & & & & 0 \end{pmatrix} \end{aligned}$$

known well that  $\mathbf{Q}_{j,j} = 1/h^2 + \varphi_0$  and  $\mathbf{p}_{i,j} = \mu(\mathbf{p}_i)$  for  $2 \leq j \leq N + 1$ :

$$\mu(\mathbf{p}_{i+1}) = \left| \frac{1/2h^2}{1/h^2 + a_0 - (1/2h^2)\mu(\mathbf{p}_i)} \right| = \frac{M^2}{2[M^2(1 - \mu(\mathbf{p}_i)/2) + a_0]}.$$

Hence, we conclude that since  $0 \leq \mu(\mathbf{p}_i) < 1$ , it means that  $\mu(\mathbf{p}_{i+1}) < 1$ . So,  $\mu(\mathbf{p}_{i+1}) < 1$  for any  $i \in [1, M]$ .

### 3.5 A New Definition of Fractional Time Derivative in Riemann–Liouville Sense

Many problems and phenomena in real life are, at a certain stage, separated from the past and to mathematically analyse their models; we do not need to step back until the instant  $t = -\infty$ . A fixed instant  $t = t_0$  is usually chosen as the starting time from which the process begins. Known assumptions on the behaviour of the function and its derivatives are given and represent the initial conditions. This results in the state of the system and contains effect of all its history. However, in classical calculus (that is, non-fractional calculus), initial conditions are constants, while the requirement for fractional calculus to give a reliable history of a physical system, especially in physics, is by nonconstant time initialization. These physical systems include, but do not limit to, semi-infinite lossy transmission line system, coloured noise, viscoelasticity, system of diffusion of heat into semi-infinite solid, dielectric polarization, electrode–electrolyte polarization, boundary layer effects in ducts and electromagnetic waves. Hence, the nonconstant initialization is the main condition for the fractional concept of integration and differentiation, since it provides the behaviour of the function before the process of differentiation–integration begins and makes the dynamics continuous after. It is widely known and proved [8–10] that the Riemann–Liouville fractional derivative satisfies this condition, while the Caputo–Fabrizio derivative encounters some challenges to get the equivalent history of the system.

It is important to mention that fractional-order initial states, as required by fractional differential equation using the Riemann–Liouville fractional derivative, are very difficult to obtain and sometimes appears to simply be physically non-realizable. In short, most of the steps in the development of the fractional calculus have ever since disregarded the issue of initialization. Liouville and Riemann, in their respective initialization, chose the lower limit to be  $-\infty$  and a real number say  $k$ , but they were in fact addressed problems relating to the same type of initialization. Caputo [11], however, opined that, to examine the composition of the fractional differintegrals, the integrated function as well as its integer-order derivatives must be equal to zero. Despite the mathematical advantage that the Caputo–Fabrizio derivative of a constant is zero and models formulated with the Caputo–Fabrizio derivative require integer-order initial conditions, there are lot of insufficiencies in the physical reality

of the initialization effects, especially when applied to fractional differential equations. Indeed, a constant initialization of the past lacks generality, as reflected in the well-known Laplace transform for differintegrals based on that assumption. This insurgency can also reflect in the solutions of fractional differential equations with histories assumed to be the set of initializing constants, representing the values of fractional differintegrals at the starting time.

To tackle some non-resolved problems related to the observable behaviour in systems of standard electromagnetic, viscoelastic materials, thermal media, and other systems mentioned above, Caputo and Fabrizio [12] proposed a new definition of fractional time derivative with no singularity  ${}_a^C \mathcal{D}_t^\alpha$ . Recall that

$$\begin{aligned} {}^{CF} \mathcal{D}_t^\alpha u(t) &= \frac{1}{\Gamma(n-\alpha)} \int_a^t \frac{1}{(t-\xi)^{1-n+\alpha}} \mathcal{D}_t^n u(\xi) d\xi, \quad \text{for } n-1 < \alpha < n \\ &= \mathcal{D}_t^n u(t) \quad \text{for } \alpha = n \end{aligned} \quad (3.5.1)$$

with  $n = 1$ , we have the Caputo version

$${}_a^C \mathcal{D}_t^\alpha u(t) = \frac{M(\alpha)}{(1-\alpha)} \int_a^t \dot{u}(\xi) \exp\left(-\frac{\alpha(t-\xi)}{1-\alpha}\right) d\xi, \quad (3.5.2)$$

where  $M(\alpha)$  remains as earlier defined. We also remark that the authors in [12] substituted the kernel  $\frac{1}{(t-\xi)^\alpha}$  appearing in (3.5.1) when  $n = 1$  by the function  $\exp\left(-\frac{\alpha(t-\xi)}{1-\alpha}\right)$ , and the term  $\frac{1}{\Gamma(1-\alpha)}$  by  $\frac{M(\alpha)}{(1-\alpha)}$ . This is done to remove the singularity issue at  $t = \xi$  that exists in the previous Caputo–Fabrizio derivative.

For a function  $u \in L^1(-\infty, b)$  we have, for  $0 \leq \alpha \leq 1$ ,

$${}_a^C \mathcal{D}_t^\alpha u(t) = \frac{\alpha M(\alpha)}{(1-\alpha)} \int_{-\infty}^t (u(t) - u(\xi)) \exp\left(-\frac{\alpha(t-\xi)}{1-\alpha}\right) d\xi. \quad (3.5.3)$$

Moreover, it is improved that

$$\lim_{\alpha \rightarrow 1} {}_a^C \mathcal{D}_t^\alpha u(t) = \dot{u}(t) \quad (3.5.4)$$

and

$$\lim_{\alpha \rightarrow 0} {}_a^C \mathcal{D}_t^\alpha u(t) = u(t) - u(\xi), \quad (3.5.5)$$

where  $a$  is the starting point of the integro-differentiation [9].

The definition of the Caputo–Fabrizio fractional derivative was also improved in [13] by Losada and Nieto as

$${}_0^C \mathcal{D}_t^\alpha u(t) = \frac{(2-\alpha)M(\alpha)}{(1-\alpha)} \int_0^t \dot{u}(\xi) \exp\left(-\frac{\alpha(t-\xi)}{1-\alpha}\right) d\xi. \quad (3.5.6)$$

Now, from the Riemann–Liouville fractional derivative with  $n = 1$ , if we carry out a similar substitution as above, we define the following derivative, considered as the new version of the Riemann–Liouville time derivative expressed for  $0 \leq \alpha \leq 1$  :

$${}_a\mathbf{D}_t^\alpha u(t) = \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} \int_a^t u(\xi) \exp\left[-\frac{\alpha}{1-\alpha}(t-\xi)\right] d\xi, \quad (3.5.7)$$

which is improved to become

$${}_a\mathbf{D}_t^\alpha u(t) = \frac{(2-\alpha)M(\alpha)}{2(1-\alpha)} \frac{d}{dt} \int_a^t u(\xi) \exp\left(-\frac{\alpha(t-\xi)}{1-\alpha}\right) d\xi. \quad (3.5.8)$$

Obviously, there is no singularity in this case at  $t = \xi$ . By following the same approach in [9, 12], we easily verify that

$$\lim_{\alpha \rightarrow 1} {}_a\mathbf{D}_t^\alpha u(t) = \dot{u}(t) \quad (3.5.9)$$

and, contrary to the Caputo–Fabrizio fractional derivative with (3.5.5), we have the exact version

$$\lim_{\alpha \rightarrow 0} {}_a\mathbf{D}_t^\alpha u(t) = u(t). \quad (3.5.10)$$

The new Riemann–Liouville fractional derivation proposed by Goufo and Atangana [9] is considered as the derivative of convolution. Recall that we can write (3.5.7) in the form

$${}_a\mathbf{D}_t^\alpha u(t) = \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} (u(t) * v(t)), \quad (3.5.11)$$

where  $v(t) = \exp\left(-\frac{\alpha t}{1-\alpha}\right)$  and  $*$  denotes the Laplace operator giving the convolution integral with two functions, which reads in classical notation

$$u(t) * v(t) = \int_a^t u(\xi) v(t-\xi) d\xi.$$

The new derivative here functions like a filter that removes the impurity left behind by modelling with other traditional derivatives.

Without loss of generality, we set  $a = 0$  and put  ${}_0\mathbf{D}_t^\alpha = \mathbf{D}_t^\alpha$ . Then, by using definition (3.5.11) and the Laplace transform properties  $\mathcal{L}(u(t)v(t), s)$ , we obtain the Laplace transform of the new fractional derivative in Riemann–Liouville sense as

$$\begin{aligned} \mathcal{L}(\mathbf{D}_t^\alpha) &= \frac{M(\alpha)}{1-\alpha} \mathcal{L}\left[\frac{d}{dt} \int_0^t u(\xi) \exp\left(-\frac{\alpha(t-\xi)}{1-\alpha}\right) d\xi, s\right] \\ &= \frac{M(\alpha)}{1-\alpha} \mathcal{L}\left(\frac{d}{dt} (u(t) * v(t)), s\right) \end{aligned}$$

$$= \frac{M(\alpha)}{1-\alpha} [s\mathcal{L}(u(t), s)\mathcal{L}(v(t), s)].$$

Hence,

$$\mathcal{L}(\mathbf{D}_t^\alpha u(t), s) = \frac{sM(\alpha)}{s + \alpha(1-s)} \mathcal{L}(f(t), s). \quad (3.5.12)$$

The main object of this section is to present the numerical approximations for the new Riemann–Liouville fractional derivative without singular kernel:

$$\mathbf{D}_t^\alpha u(t) = {}_0\mathbf{D}_t^\alpha u(t) = \frac{M(\alpha)}{1-\alpha} \frac{d}{dt} \int_0^t u(\xi) \exp\left(-\frac{\alpha(t-\xi)}{1-\alpha}\right) d\xi. \quad (3.5.13)$$

In what follows, we give the first- and second-order approximation of this new derivative.

### First-Order Approximation Method

For the finite difference scheme, let  $S \in \mathbb{N}$  be an integer which represents the grids size as

$$h = \frac{1}{S}$$

and the time grid points  $t_s = sh$  taken in the time interval  $[0, T]$  with  $s = 0, 1, 2, \dots, TS$ . We note

$$u^s = u(t_s), \quad (3.5.14)$$

the value of the function  $u$  at the grid point  $t_s$ . We make use of the following approximations:

$$\frac{dU}{dt} = \frac{U(t_{s+1}) - U(t_s)}{h} + \mathcal{O}(h) \quad \text{and} \quad U = \frac{U(t_{s+1}) + U(t_s)}{2}.$$

A discrete approximation to the new fractional derivative can be obtained as follows:

$$\begin{aligned} \mathbf{D}_t^\alpha u(t_s) = & \frac{M(\alpha)}{h(1-\alpha)} \left[ \int_0^{t_{s+1}} u(\xi) \exp\left(-\frac{\alpha}{1-\alpha}(t_{s+1}-\xi)\right) d\xi \right. \\ & \left. - \int_0^{t_s} u(\xi) \exp\left(-\frac{\alpha}{1-\alpha}(t_s-\xi)\right) d\xi + \mathcal{O}(h) \right]. \end{aligned}$$

This gives the sums

$$\begin{aligned} \mathbf{D}_t^\alpha u(t_s) = & \frac{M(\alpha)}{h(1-\alpha)} \left[ \sum_{i=1}^{s+1} \int_{(i-1)h}^{ih} \left( \frac{u^{i+1} + u^i}{2} \right) \exp\left(-\frac{\alpha}{1-\alpha}(t_{s+1}-\xi)\right) d\xi \right. \\ & \left. - \sum_{i=1}^s \int_{(i-1)h}^{ih} \left( \frac{u^{i+1} + u^i}{2} \right) \exp\left(-\frac{\alpha}{1-\alpha}(t_s-\xi)\right) d\xi + \mathcal{O}(h) \right]. \end{aligned}$$

Rearranging and integrating over the interval  $[i - 1, i]$ , we obtain

$$\mathbf{D}_t^\alpha u(t_s) = \frac{M(\alpha)}{h(1-\alpha)} \left[ \sum_{i=1}^{s+1} \left( \frac{u^{i+1} + u^i}{2} \right) \int_{(i-1)h}^{ih} \exp\left(-\frac{\alpha}{1-\alpha}(t_{s+1} - \xi)\right) d\xi - \sum_{i=1}^s \left( \frac{u^{i+1} + u^i}{2} \right) \int_{(i-1)h}^{ih} \exp\left(-\frac{\alpha}{1-\alpha}(t_s - \xi)\right) d\xi + \mathcal{O}(h) \right],$$

$$\mathbf{D}_t^\alpha u(t_s) = \frac{M(\alpha)}{\alpha h} \left[ \sum_{i=1}^{s+1} \left( \frac{u^{i+1} + u^i}{2} \right) \chi_{i,h} - \sum_{i=1}^s \left( \frac{u^{i+1} + u^i}{2} \right) \bar{\chi}_{i,h} + \mathcal{O}(h) \right],$$

where

$$\chi_{i,h} = \exp\left(-\frac{\alpha h}{1-\alpha}(s-i+1)\right) - \exp\left(-\frac{\alpha h}{1-\alpha}(s-i+2)\right), \quad (3.5.15)$$

$$\bar{\chi}_{i,h} = \exp\left(-\frac{\alpha h}{1-\alpha}(s-i)\right) - \exp\left(-\frac{\alpha h}{1-\alpha}(s-i+1)\right). \quad (3.5.16)$$

$$\mathbf{D}_t^\alpha u(t_s) = \frac{M(\alpha)}{\alpha h} \left[ \sum_{i=1}^{s+1} \left( \frac{u^{i+1} + u^i}{2} \right) \chi_{i,h} - \sum_{i=1}^s \left( \frac{u^{i+1} + u^i}{2} \right) \bar{\chi}_{i,h} \right] + \frac{M(\alpha)}{\alpha l} \mathcal{O}(h). \quad (3.5.17)$$

The following proposition is made.

**Proposition 3.5.1** *Let  $u : (a, b) \rightarrow \mathbb{R}$  an arbitrary real and locally integrable function,  $t_s \in (a, b)$  with  $\alpha \in [0, 1]$ ; then, the first-order approximation of the new Riemann–Liouville fractional derivative with no singularity kernel (3.5.13) at a point  $t_s$  is given by*

$$\mathbf{D}_t^\alpha u(t_s) = \frac{M(\alpha)}{\alpha h} \left[ \sum_{i=1}^{s+1} \left( \frac{u^{i+1} + u^i}{2} \right) \chi_{i,h} - \sum_{i=1}^s \left( \frac{u^{i+1} + u^i}{2} \right) \bar{\chi}_{i,h} \right] + \mathcal{O}(1), \quad (3.5.18)$$

where  $\chi_{i,h}$  and  $\bar{\chi}_{i,h}$  are, respectively, given in (3.5.15) and (3.5.16), and the value  $u^i$  is defined in (3.5.14).

*Proof* The proof follows directly from (3.5.17) where the term  $\frac{M(\alpha)}{\alpha h} \mathcal{O}(h)$  simply becomes  $\mathcal{O}(1)$ . □

### Second-Order Approximation Method

Here, we present a second-order numerical approximation for the new fractional derivative in Riemann–Liouville sense as

$$\mathbf{D}_{it}^\alpha u(t) = \frac{M(\alpha)}{1-\alpha} \frac{d^2}{dt^2} \int_0^t u(\xi) \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t-\xi) \right)^2 \right] d\xi, \quad (3.5.19)$$

for  $1 \leq \alpha \leq 2$ . Together with  $u = \frac{u(t_{s+1})+u(t_s)}{2}$ , we make use of the Crank–Nicholson that defines the second-order time derivative as

$$\frac{d^2 U}{dt^2} = \frac{U(t_{s+1}) - 2U(t_s) + U(t_{s-1}))}{2h^2} + \mathcal{O}(h^2).$$

As shown previously, a discrete approximation to the second-order new fractional derivative is obtained by

$$\begin{aligned} \mathbf{D}_{it}^\alpha u(t_s) &= \frac{M(\alpha)}{2h^2(1-\alpha)} \left[ \int_0^{t_{s+1}} u(\xi) \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_{s+1}-\xi) \right)^2 \right] d\xi \right. \\ &\quad - 2 \int_0^{t_s} u(\xi) \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_s-\xi) \right)^2 \right] d\xi \\ &\quad \left. + \int_0^{t_{s-1}} u(\xi) \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_{s-1}-\xi) \right)^2 \right] d\xi + \mathcal{O}(h^2) \right] \end{aligned}$$

which lead to the sums

$$\begin{aligned} \mathbf{D}_{it}^\alpha u(t_s) &= \frac{M(\alpha)}{2h^2(1-\alpha)} \left[ \sum_{i=1}^{s+1} \int_{(i-1)h}^{ih} \left( \frac{u^{i+1} + u^i}{2} \right) \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_{s+1}-\xi) \right)^2 \right] d\xi \right. \\ &\quad - 2 \sum_{i=1}^s \int_{(i-1)h}^{ih} \left( \frac{u^{i+1} + u^i}{2} \right) \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_s-\xi) \right)^2 \right] d\xi \\ &\quad \left. + \sum_{i=1}^{s-1} \int_{(i-1)h}^{ih} \left( \frac{u^{i+1} + u^i}{2} \right) \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_{s-1}-\xi) \right)^2 \right] d\xi + \mathcal{O}(h^2) \right]. \end{aligned}$$

On rearranging, we have

$$\begin{aligned} \mathbf{D}_{it}^\alpha u(t_s) &= \frac{M(\alpha)}{2h^2(1-\alpha)} \left[ \sum_{i=1}^{s+1} \left( \frac{u^{i+1} + u^i}{2} \right) \int_{(i-1)h}^{ih} \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_{s+1}-\xi) \right)^2 \right] d\xi \right. \\ &\quad - 2 \sum_{i=1}^s \left( \frac{u^{i+1} + u^i}{2} \right) \int_{(i-1)h}^{ih} \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_s-\xi) \right)^2 \right] d\xi \\ &\quad \left. + \sum_{i=1}^{s-1} \left( \frac{u^{i+1} + u^i}{2} \right) \int_{(i-1)h}^{ih} \exp \left[ - \left( \frac{\alpha}{1-\alpha} (t_{s-1}-\xi) \right)^2 \right] d\xi + \mathcal{O}(h^2) \right]. \end{aligned}$$

By integrating over the interval  $[(i-1)h, ih]$  yields

$$\mathbf{D}_{tt}^\alpha u(t_s) = \frac{\sqrt{\pi}M(\alpha)}{4\alpha h^2} \left[ \sum_{i=1}^{s+1} \left( \frac{u^{i+1} + u^i}{2} \right) \chi_{i,h} - 2 \sum_{i=1}^s \left( \frac{u^{i+1} + u^i}{2} \right) \bar{\chi}_{i,h} + \sum_{i=1}^{s-1} \left( \frac{u^{i+1} + u^i}{2} \right) \hat{\chi}_{i,h} + \mathcal{O}(h^2) \right],$$

where

$$\chi_{i,h} = \operatorname{Erf} \left[ \left( \frac{\alpha}{1-\alpha} \right) (2+s-i)h \right] - \operatorname{Erf} \left[ \left( \frac{\alpha}{1-\alpha} \right) (1+s-i)h \right], \quad (3.5.20)$$

$$\bar{\chi}_{i,h} = \operatorname{Erf} \left[ \left( \frac{\alpha}{1-\alpha} \right) (1+s-i)h \right] - \operatorname{Erf} \left[ \left( \frac{\alpha}{1-\alpha} \right) (s-i)h \right], \quad (3.5.21)$$

and

$$\hat{\chi}_{i,h} = \operatorname{Erf} \left[ \left( \frac{\alpha}{1-\alpha} \right) (s-i)h \right] - \operatorname{Erf} \left[ \left( \frac{\alpha}{1-\alpha} \right) (-1+s-i)h \right], \quad (3.5.22)$$

with  $\operatorname{Erf}[x]$  denoting the Gauss error function

$$\operatorname{Erf}[x] = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-\xi^2) d\xi.$$

Hence,

$$\mathbf{D}_{tt}^\alpha u(t_s) = \frac{\sqrt{\pi}M(\alpha)}{4\alpha h^2} \left[ \sum_{i=1}^{s+1} \left( \frac{u^{i+1} + u^i}{2} \right) \chi_{i,h} - \sum_{i=1}^s (u^{i+1} + u^i) \bar{\chi}_{i,h} + \sum_{i=1}^{s-1} \left( \frac{u^{i+1} + u^i}{2} \right) \hat{\chi}_{i,h} \right] + \frac{\sqrt{\pi}M(\alpha)}{4\alpha h^2} \mathcal{O}(h^2). \quad (3.5.23)$$

This results in the following proposition for the second-order approximation method of the new fractional derivative in Riemann–Liouville sense with no singular kernel.

**Proposition 3.5.2** *Let  $u : (a, b) \rightarrow \mathbb{R}$  an arbitrary real and locally integrable function,  $t_s \in (a, b)$  with  $\alpha \in [1, 2]$ ; then, the second-order approximation of the new Riemann–Liouville fractional derivative with no singularity kernel (3.5.13) at a point  $t_s$  is given by*

$$\mathbf{D}_{tt}^\alpha u(t_s) = \frac{\sqrt{\pi}M(\alpha)}{4\alpha h^2} \left[ \sum_{i=1}^{s+1} \left( \frac{u^{i+1} + u^i}{2} \right) \chi_{i,h} - \sum_{i=1}^s (u^{i+1} + u^i) \bar{\chi}_{i,h} + \sum_{i=1}^{s-1} \left( \frac{u^{i+1} + u^i}{2} \right) \hat{\chi}_{i,h} \right] + \mathcal{O}(1), \quad (3.5.24)$$

where  $\chi_{i,h}$  and  $\bar{\chi}_{i,h}$  are, respectively, given in (3.5.20), (3.5.21) and (3.5.22), and the value  $u^i$  is defined in (3.5.14).

*Proof* The proof follows directly from equation (3.5.23) where the term  $\frac{\sqrt{\pi}M(\alpha)}{4\alpha h^2} \mathcal{O}(h^2)$  simply becomes  $\mathcal{O}(1)$ .  $\square$

## References

1. D. Baleanu, K. Diethelm, E. Scalas, J.J. Trujillo, Models and numerical methods. World Sci. **3**, 10–16 (2012)
2. C. Li, D. Qian, Y.Q. Chen, On Riemann-Liouville and Caputo derivatives. Discret. Dyn. Nat. Soc. **2011**, 15 (2011). <https://doi.org/10.1155/2011/562494> (Article ID 562494)
3. K. Diethelm, N.J. Ford, A.D. Freed, Y. Luchko, Algorithms for the fractional calculus: a selection of numerical methods. Comput. Methods Appl. Mech. Eng. **194**, 743–773 (2005)
4. N.J. Ford, A.C. Simpson, The numerical solution of fractional differential equations: speed versus accuracy. Numer. Algorithms **26**, 333–346 (2001)
5. M.M. Meerschaert, C. Tadjeran, Finite difference approximations for fractional advection-dispersion equations. J. Computational Appl. Math. **172**, 65–77 (2004)
6. G. Jumarie, Modified Riemann-Liouville derivative and fractional Taylor series of nondifferentiable functions further results. Comput. Math. Appl. **51**, 1367–1376 (2006)
7. I. Karatay, S.R. Bayramoglu, A characteristic difference scheme for time-fractional heat equations based on the Crank-Nicholson difference schemes. Abstr. Appl. Anal. **2012**, 11 (2012). <https://doi.org/10.1155/2012/548292> (Article ID 548292)
8. R. Gorenflo, F. Mainardi, Fractional calculus: integral and differential equations of fractional order, in *Fractals and Fractional Calculus in Continuum Mechanics*, ed. by A. Carpinteri, F. Mainardi (Springer Verlag, Wien and New York, 1997), pp. 223–276
9. E.F.D. Goufo, A. Atangana, Analytical and numerical schemes for a derivative with filtering property and no singular kernel with applications to diffusion. Eur. Phys. J. **131**, 269 (2016). <https://doi.org/10.1140/epjp/i2016-16269-1>
10. I. Podlubny, *Fractional Differential Equations* (Academic Press, San Diego, 1999)
11. M. Caputo, Linear models of dissipation whose  $Q$  is almost frequency independent II. Geophys. J. R. Astron. Soc. **13**, 529–539 (1967)
12. M. Caputo, M. Fabrizio, A new definition of fractional derivative without singular kernel. Prog. Fract. Differ. Appl. **1**, 73–85 (2015)
13. J. Losada, J.J. Nieto, Properties of the new fractional derivative without singular kernel. Prog. Fract. Differ. Appl. **1**, 87–92 (2015)

# Chapter 4

## Numerical Approximation of Caputo Differentiation



The Caputo-fractional differentiation has been applied to many fields of science, technology and engineering due to their ability of including the initial conditions. The establishment of the numerical approximation is therefore possible if using the well-known integral transforms. Another advantage of this operator is based on its definition as a convolution of a derivative of a function and the power-law decay function. The numerical approximation is therefore the combination of the numerical approximation of the first or second derivative and the decomposition of an integral.

There has been significant interest in formulating some numerical schemes for the solution of time-fractional differential equations. In this chapter, we propose a new fractional Adams–Bashforth method to discretize the time Caputo derivative. The time-fractional equation is obtained from the standard parabolic partial differential equations by replacing the first-order time derivative with the Caputo derivative of order  $\alpha \in [0, 1]$ .

### 4.1 Numerical Approximation for Time Derivative

Let  $I = (a, b)$ , and  $\Delta t$  be the time step and  $nT > 0$  be an integer with  $\Delta t = T/nT$  and  $t_n = n\tau$ , for  $n = 0, 1, \dots, nT$ . The space time step is defined by  $\Delta x = (b - a)/N$ , for  $N > 0$  an integer. The space grid point  $x_i$  is given by  $x_i = 1 + i\Delta x$ , for  $i = 0, 1, 2, \dots, N$ . Given

$${}_0^C \mathcal{D}_t^\alpha u(x, t) = \frac{1}{\Gamma(1 - \alpha)} \int_0^t \frac{\partial u}{\partial \tau} u(x, \tau) (t - \tau)^{-\alpha} d\tau, \quad (4.1.1)$$

at  $t = t_n$ , we have

$$\begin{aligned}
{}_0^C \mathcal{D}_t^\alpha u(x, t_n) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_n} \frac{\partial u}{\partial \tau} u(x, \tau) (t_n - \tau)^{-\alpha} d\tau, \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \frac{u_i^{j+1} - u_i^j}{\Delta t} (t_n - t)^{-\alpha} dt \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \frac{u_i^{j+1} - u_i^j}{\Delta t} \int_{t_j}^{t_{j+1}} (t_n - t)^{-\alpha} dt \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \frac{u_i^{j+1} - u_i^j}{\Delta t} \int_{t_n - t_j}^{t_n - t_{j+1}} -y^\alpha dy \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \frac{u_i^{j+1} - u_i^j}{\Delta t} \left[ \frac{-y^{\alpha+1}}{-\alpha+1} \Big|_{t_n - t_j}^{t_n - t_{j+1}} \right] \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \frac{u_i^{j+1} - u_i^j}{\Delta t} \left\{ \frac{(n-j)^{1-\alpha} (\Delta t)^{1-\alpha}}{1-\alpha} - \frac{(n-j-1)^{1-\alpha} (\Delta t)^{1-\alpha}}{1-\alpha} \right\} \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \frac{u_i^{j+1} - U_i^j}{\Delta t} \delta_{n,j}^\alpha. \tag{4.1.2}
\end{aligned}$$

For the backward difference scheme,

$$\begin{aligned}
{}_0^C \mathcal{D}_t^\alpha u(x, t_n) &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^n \frac{u_i^j - u_i^{j-1}}{\Delta t} \int_{t_{j-1}}^{t_j} (t_n - t)^{-\alpha} dt \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^n \frac{u_i^j - u_i^{j-1}}{\Delta t} \int_{t_n - t_{j-1}}^{t_n - t_j} -y^\alpha dy \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^n \frac{u_i^j - u_i^{j-1}}{\Delta t} \left[ \frac{-y^{1-\alpha}}{1-\alpha} \right]_{t_n - t_{j-1}}^{t_n - t_j} \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^n \frac{u_i^j - u_i^{j-1}}{\Delta t} \left\{ \frac{(\Delta t)^{1-\alpha} (n-j+1)^{1-\alpha}}{1-\alpha} - \frac{(\Delta t)^{1-\alpha} (n-j)^{1-\alpha}}{1-\alpha} \right\} \\
&= \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=1}^n \left( u_i^j - u_i^{j-1} \right) \left\{ (n-j+1)^{1-\alpha} - (n-j)^{1-\alpha} \right\} \\
&= \frac{(\Delta t)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=1}^n \left( u_i^j - u_i^{j-1} \right) \delta_{n,j}^\alpha.
\end{aligned}$$

## 4.2 Numerical Approximation for Space First-Order Derivative

$${}_0^C \mathcal{D}_t^\alpha u(x, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^x (x-y)^{-\alpha} \frac{\partial}{\partial y} u(y, t) dy. \quad (4.2.1)$$

For the backward Euler method at point  $x_i$ , we have

$$\begin{aligned} {}_0^C \mathcal{D}_x^\alpha u(x_i, t_j) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{x_i} (x_i-y)^{-\alpha} \frac{\partial}{\partial y} u(y, t_j) dy \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \int_{x_{k-1}}^{x_k} (x_i-y)^{-\alpha} \frac{u_k^j - u_{k-1}^j}{\Delta x} dy \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \frac{u_k^j - u_{k-1}^j}{\Delta x} \int_{x_{k-1}}^{x_k} (x_i-y)^{-\alpha} dy \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \frac{u_k^j - u_{k-1}^j}{\Delta x} [-x^{-\alpha}]_{x_i-x_{k-1}}^{x_i-x_k} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \frac{u_k^j - u_{k-1}^j}{\Delta x} \times \\ &\quad \left\{ \frac{(\Delta x)^{1-\alpha} (i-k+1)^{1-\alpha}}{1-\alpha} - \frac{(\Delta x)^{1-\alpha} (i-k)^{1-\alpha}}{1-\alpha} \right\} \\ &= \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{i-1} (u_k^j - u_{k-1}^j) \left\{ (i-k+1)^{1-\alpha} - (i-k)^{1-\alpha} \right\} \\ &= \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{i-1} (u_k^j - u_{k-1}^j) \delta_{n,k}^\alpha. \end{aligned}$$

For central difference, at  $x_i$  we have

$$\begin{aligned} {}_0^C \mathcal{D}_x^\alpha u(x_i, t_j) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{x_i} (x_i-y)^{-\alpha} \frac{\partial}{\partial y} u(y, t_j) dy \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \int_{x_{k-1}}^{x_{k+1}} (x_i-y)^{-\alpha} \frac{u_{k+1}^j - u_{k-1}^j}{\Delta x} dy \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \frac{u_{k+1}^j - u_{k-1}^j}{\Delta x} \int_{x_{k-1}}^{x_{k+1}} (x_i-y)^{-\alpha} dy \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \frac{u_{k+1}^j - u_{k-1}^j}{\Delta x} [-x^{-\alpha}]_{x_i-x_{k-1}}^{x_i-x_{k+1}} \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^{i-1} \frac{u_{k+1}^j - u_{k-1}^j}{\Delta x} \times \\
&\quad \left\{ \frac{(\Delta x)^{1-\alpha}(i-k+1)^{1-\alpha}}{1-\alpha} - \frac{(\Delta x)^{1-\alpha}(i-k-1)^{1-\alpha}}{1-\alpha} \right\} \\
&= \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{i-1} (u_{k+1}^j - u_{k-1}^j) \left\{ (i-k+1)^{1-\alpha} - (i-k-1)^{1-\alpha} \right\} \\
&= \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{i-1} (u_{k+1}^j - u_{k-1}^j) \delta_{n,k}^\alpha.
\end{aligned}$$

For forward Euler at  $x_i$

$$\begin{aligned}
{}_0^C \mathcal{D}_x^\alpha u(x_i, t_j) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{x_i} (x_i - y)^{-\alpha} \frac{\partial}{\partial y} u(y, t_j) dy \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^i \int_{x_k}^{x_{k+1}} (x_i - y)^{-\alpha} \frac{u_{k+1}^j - u_k^j}{\Delta x} dy \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^i \frac{u_{k+1}^j - u_k^j}{\Delta x} \int_{x_k}^{x_{k+1}} (x_i - y)^{-\alpha} dy \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^i \frac{u_{k+1}^j - u_k^j}{\Delta x} [-x^{-\alpha}]_{x_i - x_k}^{x_i - x_{k+1}} \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=0}^i \frac{u_{k+1}^j - u_k^j}{\Delta x} \left\{ \frac{(\Delta x)^{1-\alpha}(i-k)^{1-\alpha}}{1-\alpha} - \frac{(\Delta x)^{1-\alpha}(i-k-1)^{1-\alpha}}{1-\alpha} \right\} \\
&= \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^i (u_{k+1}^j - u_k^j) \left\{ (i-k)^{1-\alpha} - (i-k-1)^{1-\alpha} \right\} \\
&= \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^i (u_{k+1}^j - u_k^j) \delta_{n,k}^\alpha.
\end{aligned}$$

For Crank–Nicholson method at  $x_i$

$$\begin{aligned}
{}_0^C \mathcal{D}_x^\alpha u(x_i, t_j) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{x_i} (x_i - y)^{-\alpha} \frac{\partial}{\partial y} u(y, t_j) dy \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^i \int_{x_{k-1}}^{x_{k+1}} (x_i - y)^{-\alpha} \left\{ \frac{u_{k+1}^{j+1} - u_{k-1}^{j+1}}{2\Delta x} + \frac{u_{k+1}^j - u_{k-1}^j}{2\Delta x} \right\} dy \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^i \left\{ \frac{u_{k+1}^{j+1} - u_{k-1}^{j+1}}{2\Delta x} + \frac{u_{k+1}^j - u_{k-1}^j}{2\Delta x} \right\} (x_i - y)^{-\alpha} dy \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^i \left\{ \frac{u_{k+1}^{j+1} - u_{k-1}^{j+1}}{2\Delta x} + \frac{u_{k+1}^j - u_{k-1}^j}{2\Delta x} \right\} [-x^{-\alpha}]_{x_i - x_{k+1}}^{x_i - x_{k-1}} \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^i \left\{ \frac{u_{k+1}^{j+1} - u_{k-1}^{j+1}}{2\Delta x} + \frac{u_{k+1}^j - u_{k-1}^j}{2\Delta x} \right\} \\
&\quad \times \left[ \frac{(\Delta x)^{1-\alpha}}{1-\alpha} (i-k+1)^{1-\alpha} + \frac{(\Delta x)^{1-\alpha}}{1-\alpha} (i-k)^{1-\alpha} \right] \\
&= \frac{(\Delta x)^{-\alpha}}{\Gamma(1-\alpha)} \sum_{k=1}^i \left\{ \frac{u_{k+1}^{j+1} - u_{k-1}^{j+1}}{2} + \frac{u_{k+1}^j - u_{k-1}^j}{2} \right\} [(i-k+1)^{1-\alpha} - (i-k)^{1-\alpha}] \\
&= \frac{(\Delta x)^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=1}^i \left\{ \frac{u_{k+1}^{j+1} - u_{k-1}^{j+1}}{2} + \frac{u_{k+1}^j - u_{k-1}^j}{2} \right\} \delta_{n,j}^\alpha. \tag{4.2.2}
\end{aligned}$$

### 4.3 Numerical Methods for Fractional Evolution Equations

In this section, we briefly present the fractional Euler and Adams methods that have been used for the solution of time-fractional evolution equations in one space dimension. Later, we present the new version of fractional Adams–Bashforth method with the Caputo derivative and its application to time-fractional system.

Denote by  $t_n = nh$ ,  $n = 0, 1, 2, \dots, N$ , where  $h = T/N$  is the step size, and  $N > 0$  is an integer and  $T > 0$ . Let  $u_n$  be the approximate solution of  $u(t_n)$  at  $t = t_n$ . In what follows, we introduce the numerical methods for the solution of problem.

#### 4.3.1 Fractional Euler and Adams Methods

Here, we briefly mention the fractional Euler and Adams methods.

The fractional forward and backward Euler methods are given as

$$u_{s+1} = \sum_{n=0}^{m-1} \frac{t_{s+1}^n}{n!} u_0^{(n)} + \frac{h^\alpha}{\Gamma(\alpha+1)} \sum_{n=0}^s \beta_{n,s+1} f(t_n, u_n), \tag{4.3.1}$$

and

$$u_{s+1} = \sum_{n=0}^{m-1} \frac{t_{s+1}^n}{n!} u_0^{(n)} + \frac{h^\alpha}{\Gamma(\alpha + 1)} \sum_{n=0}^s \beta_{n,s+1} f(t_{n+1}, u_{n+1}), \tag{4.3.2}$$

respectively, where  $\beta_{n,s+1} = (s - n + 1)^\alpha - (s - n)^\alpha$ .

Diethelm et al. [1] proposed the fractional Adams-type method of the form

$$u_{s+1}^\sigma = \sum_{n=0}^{m-1} \frac{t_{s+1}^n}{n!} u_0^{(n)} + \frac{h^\alpha}{\Gamma(\alpha + 1)} \sum_{n=0}^s \beta_{n,s+1} f(t_n, u_n), \tag{4.3.3}$$

$$u_{s+1} = \sum_{n=0}^{m-1} \frac{t_{s+1}^n}{n!} u_0^{(n)} + \frac{h^\alpha}{\Gamma(\alpha + 1)} \left\{ \sum_{n=0}^s \beta_{n,s+1} f(t_n, u_n) + v_{s+1,s+1} f(t_{s+1}, u_{s+1}^\sigma) \right\},$$

where

$$v_{n,s+1} = \begin{cases} s^{\alpha+1} - (s - \alpha)(s + 1)^\alpha, & n = 0, \\ (s - n + 2)^{\alpha+1} - 2(s - n + 1)^{\alpha+1} + (s - n)^{\alpha+1}, & 1 \leq n \leq s, \\ 1, & n = s + 1, \end{cases} \tag{4.3.4}$$

and  $\beta_{n,s+1}$  remains as defined above.

### 4.3.2 The New Fractional Adams–Bashforth Scheme with Caputo Derivative

We consider the fractional differential equation of the form

$${}^C \mathbf{D}_{0,t}^\alpha u(t) = f(t, u(t)), \tag{4.3.5}$$

where  ${}^C \mathbf{D}_{0,t}^\alpha u(t)$  denotes the Caputo derivative with order  $0 < \alpha < 1$ . By applying the fundamental theorem of calculus on Eq. (4.3.5), we obtain

$$u(t) - u(0) = \frac{1}{\Gamma(\alpha)} \int_0^t f(\lambda, u(\lambda))(t - \lambda)^{\alpha-1} d\lambda. \tag{4.3.6}$$

Thus at  $t = t_{n+1}$ ,  $n = 0, 1, 2, \dots$ , we obtain

$$u(t_{n+1}) - u(0) = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} f(t, u(t)) dt \tag{4.3.7}$$

and

$$u(t_n) - u(0) = \frac{1}{\Gamma(\alpha)} \int_0^{t_n} (t_n - t)^{\alpha-1} f(t, u(t)) dt. \quad (4.3.8)$$

By subtracting (4.3.8) from (4.3.7), we get

$$\begin{aligned} u(t_{n+1}) &= u(t_n) + \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} f(t, u(t)) dt \\ &\quad + \frac{1}{\Gamma(\alpha)} \int_0^{t_n} (t_n - t)^{\alpha-1} f(t, u(t)) dt. \end{aligned}$$

This implies that

$$u(t_{n+1}) = u(t_n) + A_{\alpha,1} + A_{\alpha,2}, \quad (4.3.9)$$

where

$$A_{\alpha,1} = \frac{1}{\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} f(t, u(t)) dt$$

and

$$A_{\alpha,2} = \frac{1}{\Gamma(\alpha)} \int_0^{t_n} (t_n - t)^{\alpha-1} f(t, u(t)) dt,$$

The function  $f(t, u(t))$  can be approximated using the Lagrange interpolation as

$$\begin{aligned} P(t) &\simeq \frac{t - t_{n-1}}{t_n - t_{n-1}} f(t_n, u_n) + \frac{t - t_n}{t_{n-1} - t_n} f(t_{n-1}, u_{n-1}) \\ &= \frac{f(t_n, u_n)}{h} (t - t_{n-1}) - \frac{f(t_{n-1}, u_{n-1})}{h} (t - t_n). \end{aligned} \quad (4.3.10)$$

Thus,

$$\begin{aligned} A_{\alpha,1} &= \frac{f(t_n, u_n)}{h\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} (t - t_{n-1}) dt - \frac{f(t_{n-1}, u_{n-1})}{\Gamma(\alpha)h} \\ &\quad \times \int_0^{t_{n+1}} (t_{n+1} - t)(t - t_n) dt \\ A_{\alpha,1} &= \frac{f(t_n, u_n)}{h\Gamma(\alpha)} \int_0^{t_{n+1}} u^{\alpha-1} (t_{n+1} - u - t_{n-1}) du - \frac{f(t_{n-1}, u_{n-1})}{\Gamma(\alpha)h} \\ &\quad \times \int_0^{t_{n+1}} u^{\alpha-1} (t_{n+1} - u - t_n) du \\ &= \frac{f(t_n, u_n)}{h\Gamma(\alpha)} \left\{ \frac{2ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right\} - \frac{f(t_{n-1}, u_{n-1})}{h\Gamma(\alpha)} \left\{ \frac{ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right\}. \end{aligned} \quad (4.3.11)$$

Therefore,

$$A_{\alpha,1} = \frac{f(t_n, u_n)}{h\Gamma(\alpha)} \left\{ \frac{2h}{\alpha} t_{n+1}^\alpha - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right\} - \frac{f(t_{n-1}, u_{n-1})}{h\Gamma(\alpha)} \left\{ \frac{h}{\alpha} t_{n+1}^\alpha - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right\}. \quad (4.3.12)$$

Similarly, we obtain

$$\begin{aligned} A_{\alpha,2} &= \frac{f(t_n, u_n)}{h\Gamma(\alpha)} \int_0^{t_n} (t_n - t)^{\alpha-1} (t - t_{n-1}) dt - \frac{f(t_{n-1}, u_{n-1})}{h\Gamma(\alpha)} \\ &\quad \times \int_0^{t_n} (t_n - t)^{\alpha-1} (t - t_n) dt \\ &= \frac{f(t_n, u_n)}{h\Gamma(\alpha)} \int_0^{t_n} u^{\alpha-1} \{t_n - u - t_{n-1}\} du + \frac{f(t_{n-1}, u_{n-1})}{h\Gamma(\alpha)} \frac{t_n^{\alpha+1}}{\alpha} \\ &= \frac{f(t_n, u_n)}{h\Gamma(\alpha)} \left\{ \frac{ht_n^\alpha}{\alpha} - \frac{t_n^{\alpha+1}}{\alpha+1} \right\} + \frac{f(t_{n-1}, u_{n-1})}{h\Gamma(\alpha+1)} t_n^{\alpha+1}. \end{aligned} \quad (4.3.13)$$

Thus the approximate solution is given as

$$\begin{aligned} u(t_{n+1}) &= u(t_n) + \frac{f(t_n, u_n)}{h\Gamma(\alpha)} \left\{ \frac{2h}{\alpha} t_{n+1}^\alpha - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} + \frac{h}{\alpha} t_n^\alpha - \frac{t_n^{\alpha+1}}{\alpha} \right\} \\ &\quad + \frac{f(t_{n-1}, u_{n-1})}{h\Gamma(\alpha)} \left\{ \frac{h}{\alpha} t_{n+1}^\alpha - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} + \frac{t_n^\alpha}{\alpha+1} \right\}. \end{aligned} \quad (4.3.14)$$

$$\begin{aligned} u(t_{n+1}) &= u(t_n) + \frac{f(t_n, u_n)}{h\Gamma(\alpha)} h^{\alpha+1} \left\{ \frac{2(n+1)^\alpha + n^\alpha}{\alpha} - \frac{(n+1)^{\alpha+1} + n^{\alpha+1}}{\alpha+1} \right\} \\ &\quad + \frac{f(t_{n-1}, u_{n-1})}{h\Gamma(\alpha)} h^{\alpha+1} \left\{ \frac{(n+1)^{\alpha+1}}{\alpha} - \frac{(n+1)^{\alpha+1}}{\alpha+1} + \frac{n^{\alpha+1}}{\alpha+1} \right\}. \end{aligned} \quad (4.3.15)$$

### 4.3.3 Existence and Uniqueness of Solutions

Let  $B = C_{a,b}$  be the Banach space of every continuous real function bounded in a closed set  $[a, b]$ , which also contains the sub-norm, and  $S$  be the shaft given as  $S = \{u, v, w \in S, u(x, t) \geq 0, v(x, t) \geq 0 \text{ and } w(x, t) \geq 0, a \leq t \leq b\}$ .

**Definition 4.3.1** Let  $\mathcal{B}$  be real Banach space with a cone, say  $P$  which has a restricted order  $\leq$  in  $\mathcal{B}$  in succeeding approach

$$x \leq y \Rightarrow y - x \in P, \quad x \leq z \Rightarrow z - x \in P.$$

For every  $x, y, z \in \mathcal{B}$ , the order interval is given as  $\langle a, b \rangle = \{f \in \mathcal{B} : a \leq f \leq b\}$ . A cone  $K$  is denoted normal if it is possible to obtain a constant  $j > 0$  such that  $p, q \in K, \Psi < p < q \Rightarrow \|p\| \leq \|q\|$ , where  $\Psi$  stands for the zeros of  $K$ .

To examine the existence of solution, we consider the following fractional system with Caputo derivative operator:

$$\begin{aligned} {}^C D_{0,t}^\alpha u(t) &= \rho(v(t) - u(t)), \\ {}^C D_{0,t}^\alpha v(t) &= (\kappa - \rho)u(t) + \kappa v(t) - \delta u(t)v(t), \\ {}^C D_{0,t}^\alpha w(t) &= -\phi w(t) + \epsilon v^2(t). \end{aligned} \tag{4.3.16}$$

By using the fundamental theorem of calculus on the above system, we have

$$\begin{aligned} u(t) - u(0) &= \frac{1}{\Gamma(\alpha)} \int_0^t \rho(v(\tau) - u(\tau))(t - \tau)^{\alpha-1} d\tau \\ v(t) - v(0) &= \frac{1}{\Gamma(\alpha)} \int_0^t ((\kappa - \rho)u(\tau) + \kappa v(\tau) - \delta u(\tau)v(\tau)) (t - \tau)^{\alpha-1} d\tau \\ w(t) - w(0) &= \frac{1}{\Gamma(\alpha)} \int_0^t (-\phi w(\tau) + \epsilon v^2(\tau)) (t - \tau)^{\alpha-1} d\tau. \end{aligned}$$

Next, we create a compact  $C_{a,b}$ , that is,

$$C_{a,b} = I_a(t_0) \times B_b(\xi),$$

where

$$\xi = \min\{u_0, v_0, w_0\}$$

and

$$I_a(t_0) = [t_0 - a, t_0 + a], \quad B_b(\xi) = [\xi - b, \xi + b].$$

Let

$$\begin{aligned} f_1(u, v, w, t) &= \rho(v(t) - u(t)), \\ f_2(u, v, w, t) &= (\kappa - \rho)u(t) + \kappa v(t) - \delta u(t)v(t), \\ f_3(u, v, w, t) &= -\phi w(t) + \epsilon v^2(t). \end{aligned} \tag{4.3.17}$$

Also, we assume

$$M = \max_{C_{a,b}} \left\{ \sup_{C_{a,b}} \|f_1\|, \sup_{C_{a,b}} \|f_2\|, \sup_{C_{a,b}} \|f_3\| \right\}.$$

By adopting the infinite norm, we have

$$\|\varphi\|_\infty = \sup_{t \in I_a} |\varphi(t)|.$$

Next, we create a function, say

$$\Gamma : C_{a,b} \rightarrow C_{a,b}$$

so that

$$\Gamma X(t) = X_0 + \frac{1}{\Gamma(\alpha)} \int_0^t F(u, v, w, t)(t - \tau)^{\alpha-1} d\tau \quad (4.3.18)$$

$$X(t) = \begin{pmatrix} u(t) \\ v(t) \\ w(t) \end{pmatrix}, \quad F(u, v, w, t) = \begin{pmatrix} f_1(u, v, w, t) \\ f_2(u, v, w, t) \\ f_3(u, v, w, t) \end{pmatrix}. \quad (4.3.19)$$

We must show that the new fractional operator is well defined, that is, we evaluate the condition for which

$$\|\Gamma X(t) - X_0\|_\infty < \begin{pmatrix} b \\ b \\ b \end{pmatrix},$$

where

$$\|\Gamma_1 u(t) - u_0\|_\infty < b,$$

$$\|\Gamma_2 v(t) - v_0\|_\infty < b,$$

$$\|\Gamma_3 w(t) - w_0\|_\infty < b.$$

Starting with the  $u$  component, we have

$$\begin{aligned} \|\Gamma_1 u(t) - u_0\|_\infty &= \left\| \frac{1}{\Gamma(\alpha)} \int_0^t f_1(u, v, w, \tau)(t - \tau)^{\alpha-1} d\tau \right\|_\infty \\ &\leq \frac{1}{\Gamma(\alpha)} \int_0^t \|f_1(u, v, w, \tau)\|_\infty (t - \tau)^{\alpha-1} d\tau \\ &\leq \frac{M}{\Gamma(\alpha)} \int_0^t (t - \tau) d\tau \\ &\leq \frac{Ma^\alpha}{\Gamma(\alpha + 1)} < b, \end{aligned} \quad (4.3.20)$$

where

$$a < \left( \frac{b\Gamma(\alpha + 1)}{M} \right)^{1/\alpha}.$$

Similarly, for the remaining components, we have

$$\|\Gamma_2 v(t) - v_0\|_\infty < \frac{Ma^\alpha}{\Gamma(\alpha + 1)}$$

and

$$\|\Gamma_3 w(t) - w_0\|_\infty < \frac{Ma^\alpha}{\Gamma(\alpha + 1)}.$$

Thus,

$$\|\Gamma X(t) - X_0\|_\infty \leq \frac{Ma^\alpha}{\Gamma(\alpha + 1)},$$

$\Gamma$  is well defined if  $a < \left(\frac{b\Gamma(\alpha+1)}{M}\right)^{1/\alpha}$ .

Second, we require to show that our function has a Lipschitz condition. That is,

$$\begin{aligned} & \|\Gamma X_1 - \Gamma X_2\|_\infty < K \|X_1 - X_2\| \\ \|\Gamma_1 u_1 - \Gamma_1 u_2\|_\infty &= \left\| \frac{1}{\Gamma(\alpha)} \int_0^t f_1(u_1, v, w, \tau)(t - \tau)^{\alpha-1} d\tau \right. \\ & \quad \left. - \frac{1}{\Gamma(\alpha)} \int_0^t f_1(u_2, v, w, \tau)(t - \tau)^{\alpha-1} d\tau \right\|_\infty \\ &= \frac{1}{\Gamma(\alpha)} \left\| \int_0^t (f_1(u_1, v, w, \tau) - f_1(u_2, v, w, \tau))(t - \tau)^{\alpha-1} d\tau \right\|_\infty \\ &\leq \frac{1}{\Gamma(\alpha)} \int_0^t \|(f_1(u_1, v, w, \tau) - f_1(u_2, v, w, \tau))\|_\infty (t - \tau)^{\alpha-1} d\tau \\ &\leq \frac{1}{\Gamma(\alpha)} \int_0^t \|(\rho v - \rho u_1 - \rho v + \rho u_2)\|_\infty (t - \tau)^{\alpha-1} d\tau \\ &\leq \frac{|\rho|}{\Gamma(\alpha)} \int_0^t \|u_1 - u_2\|_\infty (t - \tau)^{\alpha-1} d\tau \\ &< \frac{|\rho|}{\Gamma(\alpha)} \|u_1 - u_2\|_\infty \cdot \frac{a^\alpha}{\alpha} \\ &\leq \frac{|\rho| \|u_1 - u_2\|_\infty \cdot a^\alpha}{\Gamma(\alpha + 1)} \leq \|u_1 - u_2\|_\infty K_1, \end{aligned} \tag{4.3.21}$$

where

$$K_1 = \frac{|\rho|a^\alpha}{\Gamma(\alpha + 1)}.$$

Also,

$$\begin{aligned}
\|\Gamma_2 v_1 - \Gamma_2 v_2\|_\infty &= \left\| \frac{1}{\Gamma(\alpha)} \int_0^t f_2(u, v_1, w, \tau)(t - \tau)^{\alpha-1} d\tau \right. \\
&\quad \left. - \frac{1}{\Gamma(\alpha)} \int_0^t f_2(u, v_2, w, \tau)(t - \tau)^{\alpha-1} d\tau \right\|_\infty \\
&= \frac{1}{\Gamma(\alpha)} \left\| \int_0^t (f_2(u, v_1, w, \tau) - f_2(u, v_2, w, \tau)) (t - \tau)^{\alpha-1} d\tau \right\|_\infty \\
&\leq \frac{1}{\Gamma(\alpha)} \int_0^t \|(f_2(u, v_1, w, \tau) - f_2(u, v_2, w, \tau))\|_\infty (t - \tau)^{\alpha-1} d\tau \\
&\leq \frac{1}{\Gamma(\alpha)} \int_0^t \|\kappa(v_1 - v_2) - \delta u(v_1 - v_2)\|_\infty (t - \tau)^{\alpha-1} d\tau \\
&\leq \frac{1}{\Gamma(\alpha)} \int_0^t \{\kappa\|v_1 - v_2\|_\infty + \delta\|u(t)\|_\infty\|v_1 - v_2\|_\infty\} (t - \tau)^{\alpha-1} d\tau \\
&\leq \frac{(|\kappa| + |\delta|\|u(t)\|_\infty)\|v_1 - v_2\|_\infty}{\Gamma(\alpha + 1)} \cdot a^\alpha \\
&= K_2\|v_1 - v_2\|_\infty,
\end{aligned} \tag{4.3.22}$$

where

$$K_2 = \frac{(|\kappa| + |\delta|\|u(t)\|_\infty) a^\alpha}{\Gamma(\alpha + 1)}.$$

For the third component,

$$\begin{aligned}
\|\Gamma_3 w_1 - \Gamma_3 w_2\|_\infty &= \left\| \frac{1}{\Gamma(\alpha)} \int_0^t f_3(u, v, w_1, \tau)(t - \tau)^{\alpha-1} d\tau \right. \\
&\quad \left. - \frac{1}{\Gamma(\alpha)} \int_0^t f_3(u, v, w_2, \tau)(t - \tau)^{\alpha-1} d\tau \right\|_\infty \\
&= \frac{1}{\Gamma(\alpha)} \left\| \int_0^t (f_3(u, v, w_1, \tau) - f_3(u, v, w_2, \tau)) (t - \tau)^{\alpha-1} d\tau \right\|_\infty \\
&\leq \frac{1}{\Gamma(\alpha)} \int_0^t \|(f_3(u, v, w_1, \tau) - f_3(u, v, w_2, \tau))\|_\infty (t - \tau)^{\alpha-1} d\tau \\
&\leq \frac{1}{\Gamma(\alpha)} \int_0^t \|\phi(w_2 - w_1)\|_\infty (t - \tau)^{\alpha-1} d\tau \\
&\leq \frac{1}{\Gamma(\alpha)} \int_0^t \{\phi\|w_2 - w_1\|_\infty\} (t - \tau)^{\alpha-1} d\tau \\
&\leq \frac{(|\phi|\|w_2 - w_1\|) a^\alpha}{\Gamma(\alpha + 1)} \\
&\leq K_3\|w_2 - w_1\|,
\end{aligned} \tag{4.3.23}$$

where

$$\frac{|\phi|a^\alpha}{\Gamma(\alpha + 1)}.$$

So,  $\Gamma$  is a contraction if

$$\begin{pmatrix} K_1 \\ K_2 \\ K_3 \end{pmatrix} < \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = 0, \tag{4.3.24}$$

for

$$a < \left(\frac{\Gamma(\alpha + 1)}{b}\right)^{1/\alpha}, \quad a < \left(\frac{\Gamma(\alpha + 1)}{|\rho|}\right)^{1/\alpha}, \quad a < \left(\frac{\Gamma(\alpha + 1)}{|\kappa| + |\delta|\|u(t)\|_\infty}\right)^{1/\alpha}.$$

So to obtain a contraction,

$$a < \min \left\{ \left(\frac{\Gamma(\alpha + 1)}{b}\right)^{1/\alpha}, \left(\frac{\Gamma(\alpha + 1)}{|\rho|}\right)^{1/\alpha}, \left(\frac{\Gamma(\alpha + 1)}{|\kappa| + |\delta|\|u(t)\|_\infty}\right)^{1/\alpha} \right\}.$$

Under this condition,  $\Gamma$  is a contraction in a compact Banach space; this implies that  $\Gamma$  has a unique solution. For the general existence and uniqueness theorem, readers are referred to some classical books [2–4].

## References

1. K. Diethelm, N.J. Ford, A.D. Freed, Y. Luchko, Algorithms for the fractional calculus: a selection of numerical methods. *Comput. Methods Appl. Mech. Eng.* **194**, 743–773 (2005)
2. K. Diethelm, *The Analysis of Fractional Differential Equations: An Application-oriented Exposition using Differential Operators of Caputo type* (Springer Lecture Notes in Mathematics, Springer, Berlin, Heidelberg, 2010)
3. I. Podlubny, *Fractional Differential Equations* (Academic Press, San Diego, 1999)
4. S. Samko, A. Kilbas, O. Marichev, *Fractional Integrals and Derivatives: Theory and Applications* (Gordon and Breach, Amsterdam, 1993)

# Chapter 5

## Numerical Approximation of Caputo–Fabrizio Differentiation



Most fractional differential equations describing real-world (physical) problems are highly complicated and cannot sometimes be solved analytically. A lot of numerical approaches in connection with derivatives of fractional order describing these real-world problems alter essentially in the many in which the derivative of fractional order is tailored, see, for instance, [5] and references therein. Numerical approximation of a derivative of fractional order has a highly complicated formula compared to those of integer order due to their non-local nature, and therefore the calculation at a particular point requires knowledge of the function further out of the region close to that point. Accordingly, finite difference approximations of derivatives of fractional order engage a quantity of points that alters according to how faraway we are from the borderline.

One of the most recent fractional-order derivatives was proposed by Caputo and Fabrizio [3, 4], where it was shown that the new-fangled derivative contains additional encouraging properties in comparison with the older version. For example, they have shown that it can represent substance heterogeneities and configurations with different scales, which clearly cannot be overseen with the prominent local theories and also the known fractional derivative. Another application is in the investigation of the macroscopic behaviours of some materials that are associated with non-local communications between atoms, which are recognized to be important of the properties of material.

### 5.1 Numerical Approximation for the Caputo–Fabrizio Fractional Derivative in Caputo Sense

We start by presenting the numerical approximation based on the definition of the Caputo–Fabrizio derivative for Caputo-type [3, 4],

$${}_0^{CF}\mathcal{D}_t^\alpha(f(t)) = \frac{M(\alpha)}{1-\alpha} \int_0^t f'(\xi) \exp\left[-\alpha \frac{t-\xi}{1-\alpha}\right] d\xi. \quad (5.1.1)$$

For some integer  $N > 0$ , the grid size in time for finite difference technique is given by

$$k = \frac{1}{N}.$$

In the time interval  $[0, T]$ , the grid points are denoted as  $t_n = nk$ ,  $n = 0, 1, 2, \dots, TN$ . The value of the function  $f$  at the grid point is  $f_i = f(t_i)$ .

A discrete approximation to the Caputo–Fabrizio derivative of fractional order is given by the simple quadrature formula as

$${}_0^{CF}\mathcal{D}_t^\alpha(f(t_n)) = \frac{M(\alpha)}{1-\alpha} \int_0^{t_n} f'(\xi) \exp\left[-\alpha \frac{t_n-\xi}{1-\alpha}\right] d\xi. \quad (5.1.2)$$

This equation can be modified using the first-order approximation to

$${}_0^{CF}\mathcal{D}_t^\alpha(f(t_j)) = \frac{M(\alpha)}{1-\alpha} \sum_{j=1}^n \int_{(j-1)k}^{jk} \left( \frac{f^{k+1} - f^k}{\Delta t} + \mathcal{O}(\Delta t) \right) \exp\left[-\alpha \frac{t_j - \xi}{1-\alpha}\right] d\xi. \quad (5.1.3)$$

Before integrating the above, we quickly obtain the following expression:

$$\frac{M(\alpha)}{1-\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{\Delta t} + \mathcal{O}(\Delta t) \right) \int_{(j-1)k}^{jk} \exp\left[-\alpha \frac{t_j - \xi}{1-\alpha}\right] d\xi. \quad (5.1.4)$$

$${}_0^{CF}\mathcal{D}_t^\alpha(f(t_j)) = \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{\Delta t} + \mathcal{O}(\Delta t) \right) d_{j,k},$$

where

$$d_{j,k} = \exp\left[-\alpha \frac{k}{1-\alpha}(n-j+1)\right] - \exp\left[-\alpha \frac{k}{1-\alpha}(n-j)\right]. \quad (5.1.5)$$

We finally obtain

$${}_0^{CF}\mathcal{D}_t^\alpha(f(t_n)) = \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{\Delta t} \right) d_{j,k} + \frac{M(\alpha)}{\alpha} \sum_{j=1}^n d_{j,k} \mathcal{O}(\Delta t). \quad (5.1.6)$$

In the following results, we present the first-order approximations of the Caputo–Fabrizio derivative in both space and time.

**Theorem 5.1.1** Let  $f(x)$  be a function in  $C^2[a, b]$  and let the order of the fractional derivative be  $0 < \alpha \leq 1$ , then the first-order approximation of the Caputo–Fabrizio derivative in the sense of Caputo at a point  $t_n$  is given by [1]

$${}_0^{CF} \mathcal{D}_t^\alpha (f(t_n)) = \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{\Delta t} \right) d_{j,k} + \mathcal{O}((\Delta t)^2). \quad (5.1.7)$$

*Proof* From above (5.1.5), we have

$$\begin{aligned} {}_0^{CF} \mathcal{D}_t^\alpha (f(t_n)) &= \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{\Delta t} \right) d_{j,k} \\ &+ \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \exp \left[ -\alpha \frac{k}{1-\alpha} (n-j+1) \right] - \exp \left[ -\alpha \frac{k}{1-\alpha} (n-j) \right] \right) \mathcal{O}(\Delta t). \end{aligned}$$

However,

$$\begin{aligned} &\sum_{j=1}^n \left( \exp \left[ -\alpha \frac{k}{1-\alpha} (n-j+1) \right] - \exp \left[ -\alpha \frac{k}{1-\alpha} (n-j) \right] \right) \\ &= \exp \left[ -\alpha \frac{k}{1-\alpha} (n) \right] - 1. \end{aligned} \quad (5.1.8)$$

Approximation of the exponential function is obtained as

$$\exp \left[ -\alpha \frac{k}{1-\alpha} (n) \right] \approx 1 - \alpha \frac{k}{1-\alpha} (n).$$

This function is replaced in (5.1.8) to yield

$$\sum_{j=1}^n \left( \exp \left[ -\alpha \frac{k}{1-\alpha} (n-j+1) \right] - \exp \left[ -\alpha \frac{k}{1-\alpha} (n-j) \right] \right) \approx -\alpha \frac{k}{1-\alpha} (n). \quad (5.1.9)$$

Then Eq. (5.1.8) results in

$${}_0^{CF} \mathcal{D}_t^\alpha (f(t_n)) = \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{\Delta t} \right) d_{j,k} + \frac{M(\alpha)k}{1-\alpha} (n) \mathcal{O}(\Delta t). \quad (5.1.10)$$

And the requested result is obtained as

$${}_0^{CF}\mathcal{D}_t^\alpha(f(t_n)) = \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{\Delta t} \right) d_{j,k} + \mathcal{O}((\Delta t)^2). \quad (5.1.11)$$

The proof is completed.  $\square$

We now conclude that the first-order approximation scheme for the computation of the time-fractional-order Caputo–Fabrizio derivative in the sense of Caputo is given as

$${}_0^{CF}\mathcal{D}_t^\alpha(f(t_n)) = \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{\Delta t} \right) d_{j,k}. \quad (5.1.12)$$

Next, we present the numerical approximation for first-order space Caputo–Fabrizio derivative in Caputo sense.

Consider some integer  $N > 0$ , the grid sizes in time for finite difference technique are defined by

$$i = \frac{1}{M}.$$

The grid points in the time interval  $[0, X]$  are denoted  $x_i = im$ ,  $m = 0, 1, 2, \dots, XM$ . The value of the function  $f$  at the points is given as  $f_i^k = f(x_i, t_k)$ . We obtain

$${}_0^{CF}\mathcal{D}_t^\alpha(f(x_m, t_i)) = \frac{M(\alpha)}{\sqrt{\pi}(1-\alpha)} \int_0^{x_m} \frac{\partial}{\partial \tau} f'(\tau, t_i) \exp \left[ -\alpha^2 \frac{(x_m - \tau)^2}{(1-\alpha)^2} \right] d\tau.$$

By employing the Crank–Nicholson approximation for the first-order derivative, the above equation is transformed into

$$\begin{aligned} {}_0^{CF}\mathcal{D}_x^\alpha(f(x_m, t_k)) &= \frac{M(\alpha)}{\sqrt{\pi}(1-\alpha)} \int_0^{x_m} \left( \frac{(f_{i+1}^{k+1} - f_{i-1}^{k+1}) - (f_{i+1}^k - f_{i-1}^k)}{4\Delta x} + \mathcal{O}(\Delta t) \right) \\ &\times \exp \left[ -\alpha^2 \frac{(x_m - \tau)^2}{(1-\alpha)^2} \right] d\tau. \end{aligned} \quad (5.1.13)$$

The above equation is converted to

$$\begin{aligned} {}_0^{CF}\mathcal{D}_x^\alpha(f(x_m, t_i)) &= \frac{M(\alpha)}{\sqrt{\pi}(1-\alpha)} \sum_{s=1}^m \left\{ \frac{(f_{s+1}^{k+1} - f_{s-1}^{k+1}) - (f_{s+1}^k - f_{s-1}^k)}{4\Delta x} + \mathcal{O}(i) \right\} \\ &\times \int_{(s-1)i}^{si} \exp \left[ -\alpha^2 \frac{(im - \tau)^2}{(1-\alpha)^2} \right] d\tau, \end{aligned} \quad (5.1.14)$$

and the integral part is defined as

$$\int_{(s-1)i}^{si} \exp \left[ -\alpha^2 \frac{(im - \tau)^2}{(1 - \alpha)^2} \right] d\tau = \frac{(1 - \alpha)\sqrt{\pi}}{2\alpha} \left\{ \operatorname{erf} \left[ (mi - si) \frac{\alpha}{1 - \alpha} \right] - \operatorname{erf} \left[ (mi - si + i) \frac{\alpha}{1 - \alpha} \right] \right\},$$

in such a way that (5.1.11) becomes

$$\begin{aligned} {}_0^{CF} \mathcal{D}_x^\alpha (f(x_m, t_k)) &= \frac{M(\alpha)}{1 - \alpha} \sum_{s=1}^m \left\{ \frac{(f_{s+1}^{k+1} - f_{s-1}^{k+1}) - (f_{s+1}^k - f_{s-1}^k)}{4\Delta x} + \mathcal{O}(i) \right\} \\ &\times \frac{(1 - \alpha)}{2\alpha} \left\{ \operatorname{erf} \left[ (m - s) \frac{\alpha i}{1 - \alpha} \right] - \operatorname{erf} \left[ (m - s + 1) \frac{\alpha i}{1 - \alpha} \right] \right\}. \end{aligned} \quad (5.1.15)$$

From (5.1.15), we have

$$\begin{aligned} {}_0^{CF} \mathcal{D}_x^\alpha (f(x_m, t_k)) &= \frac{M(\alpha)}{1 - \alpha} \sum_{s=1}^m \left\{ \frac{(f_{s+1}^{k+1} - f_{s-1}^{k+1}) - (f_{s+1}^k - f_{s-1}^k)}{4\Delta x} \frac{(1 - \alpha)\sqrt{\pi}}{2\alpha} \right. \\ &\times \left. \left\{ \operatorname{erf} \left[ (m - s) \frac{\alpha i}{1 - \alpha} \right] - \operatorname{erf} \left[ (m - s + 1) \frac{\alpha i}{1 - \alpha} \right] \right\} \right\} \\ &+ \mathcal{O}(i) \frac{(1 - \alpha)}{2\alpha} \left\{ \operatorname{erf} \left[ (m - s) \frac{\alpha i}{1 - \alpha} \right] - \operatorname{erf} \left[ (m - s + 1) \frac{\alpha i}{1 - \alpha} \right] \right\}. \end{aligned} \quad (5.1.16)$$

**Theorem 5.1.2** Let  $f(x, t)$  be a function in  $C^2([a, b] \times [0, T])$ , and let the order of the fractional derivative be  $0 < \alpha \leq 1$ . Then the first-order approximation of the Caputo–Fabrizio derivative in Caputo sense at a point  $(x_m, t_n)$  is

$${}_0^{CF} \mathcal{D}_x^\alpha (f(x_m, t_k)) = \frac{M(\alpha)}{2\alpha} \sum_{s=1}^m \left\{ \frac{(f_{s+1}^{k+1} - f_{s-1}^{k+1}) - (f_{s+1}^k - f_{s-1}^k)}{4\Delta x} \right\} d_{i,s} + E(\alpha, i, s), \quad (5.1.17)$$

where

$$d_{i,s} = \left\{ \operatorname{erf} \left[ (m - s) \frac{\alpha i}{1 - \alpha} \right] - \operatorname{erf} \left[ (m - s + 1) \frac{\alpha i}{1 - \alpha} \right] \right\}, \quad \|E(\alpha, i, l)\| < M.$$

*Proof* From (5.1.17), we have

$$\begin{aligned} {}_0^{CF} \mathcal{D}_x^\alpha (f(x_m, t_k)) &= \frac{M(\alpha)}{2\alpha} \sum_{s=1}^m \left\{ \frac{(f_{s+1}^{k+1} - f_{s-1}^{k+1}) - (f_{s+1}^k - f_{s-1}^k)}{4\Delta x} \right. \\ &\times \left. \left\{ \operatorname{erf} \left[ (m - s) \frac{\alpha i}{1 - \alpha} \right] - \operatorname{erf} \left[ (m - s + 1) \frac{\alpha i}{1 - \alpha} \right] \right\} \right\} \\ &+ \mathcal{O}(i) \frac{M(\alpha)}{2\alpha} \sum_{s=1}^m \left\{ \operatorname{erf} \left[ (m - s) \frac{\alpha i}{1 - \alpha} \right] - \operatorname{erf} \left[ (m - s + 1) \frac{\alpha i}{1 - \alpha} \right] \right\}. \end{aligned}$$

We let

$$E(\alpha, i, s) = \mathcal{O}(i) \frac{M(\alpha)}{2\alpha} \sum_{s=1}^m \left\{ \operatorname{erf} \left[ (m-s) \frac{\alpha i}{1-\alpha} \right] - \operatorname{erf} \left[ (m-s+1) \frac{\alpha i}{1-\alpha} \right] \right\}.$$

On taking the norm to both sides, we have

$$\begin{aligned} \|E(\alpha, i, s)\| &= \left\| \mathcal{O}(i) \frac{M(\alpha)}{2\alpha} \sum_{s=1}^m \left\{ \operatorname{erf} \left[ (m-s) \frac{\alpha i}{1-\alpha} \right] \right. \right. \\ &\quad \left. \left. - \operatorname{erf} \left[ (m-s+1) \frac{\alpha i}{1-\alpha} \right] \right\} \right\|, \end{aligned} \quad (5.1.18)$$

$$\|E(\alpha, i, s)\| = \left\| \mathcal{O}(i) \frac{M(\alpha)}{2\alpha} \left( \operatorname{erf} \left[ m \frac{-\alpha i}{1-\alpha} \right] \right) \right\|.$$

This completes the proof.  $\square$

Then, the first-order approximation method for the computation of Caputo–Fabrizio derivative of space-fractional order in Caputo sense is given as

$$\begin{aligned} {}_0^{CF} \mathcal{D}_x^\alpha (f(x_m, t_k)) &= \frac{M(\alpha)}{2\alpha} \sum_{s=1}^m \left\{ \frac{(f_{s+1}^{k+1} - f_{s-1}^{k+1}) - (f_{s+1}^k - f_{s-1}^k)}{4\Delta x} \right. \\ &\quad \left. \times \left\{ \operatorname{erf} \left[ (m-s) \frac{\alpha i}{1-\alpha} \right] - \operatorname{erf} \left[ (m-s+1) \frac{\alpha i}{1-\alpha} \right] \right\} \right\}. \end{aligned} \quad (5.1.19)$$

Due to the known fact that there are some physical problems that cannot be modelled by the power law, as a result, Caputo and Fabrizio in their joint work [3] suggested an alternative concept of differentiation with the use of the exponential decay as kernel instead of the power law. This new differentiation approach which has caught many scholars was also disqualified to be classified as a fractional derivative due to the fact that the kernel was not non-local; however, it is clear that many physical problems encountered in science and engineering conformed with the exponential decay law which indeed has no singularity which makes this derivative useful in modelling such real-world problems.

## 5.2 Numerical Approximation for Time Derivative

The numerical approximation of the version suggested by Caputo and Fabrizio was also suggested by Atangana and Nieto. In this work, we pay attention to the numerical approximation on the version suggested in [1]. We begin by presenting the time derivative, by definition as in [2]

$$\begin{aligned}
U(t) &= \frac{M(\alpha)}{1-\alpha} \int_0^t \exp\left(-\frac{\alpha}{1-\alpha}(t-\tau)\right) f(\tau) d\tau, \\
{}^R\mathcal{D}_t^\alpha\{f(t)\} &= \frac{d}{dt}U(t), \\
\frac{d}{dt}U(t) &= \frac{U(t_{j+1}) - U(t_j)}{\Delta t} + \mathcal{O}(\Delta t), \\
U(t_{j+1}) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{j+1}} f(\tau) \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1}-\tau)\right) d\tau, \\
U(t_j) &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_j} f(\tau) \exp\left(-\frac{\alpha}{1-\alpha}(t_j-\tau)\right) d\tau.
\end{aligned} \tag{5.2.1}$$

Without loss of generality, the full approximation is presented as follows:

$$\begin{aligned}
u(t_{j+1}) &= \frac{M(\alpha)}{1-\alpha} \int_0^{t_{j+1}} f(\tau) \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1}-\tau)\right) d\tau, \\
&= \frac{M(\alpha)}{1-\alpha} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \frac{f(t_{s+1}) + f(t_s)}{2} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1}-\tau)\right) d\tau + H_1, \\
&= \frac{M(\alpha)}{1-\alpha} \sum_{s=0}^j \frac{f(t_{s+1}) + f(t_s)}{2} \int_{t_s}^{t_{s+1}} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1}-\tau)\right) d\tau + H_1 \\
&= \frac{M(\alpha)}{\alpha} \sum_{s=0}^j \frac{f(t_{s+1}) + f(t_s)}{2} \left\{ \exp\left(-\alpha \frac{t_{j+1}-t_{s+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_{j+1}-t_s}{1-\alpha}\right) \right\} + H_1, \\
&= \frac{M(\alpha)}{\alpha} \sum_{s=0}^j \frac{f(t_{s+1}) + f(t_s)}{2} \delta_{j,s}^\alpha + H_1,
\end{aligned} \tag{5.2.2}$$

where

$$\delta_{j,s}^\alpha = \exp\left(-\alpha \frac{t_{j+1}-t_{s+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_{j+1}-t_s}{1-\alpha}\right), \tag{5.2.3}$$

and

$$H_1 = \frac{M(\alpha)}{1-\alpha} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \{f(\nu) - f(t_{s+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1}-\tau)\right) d\nu. \tag{5.2.4}$$

Similarly, we obtain

$$\begin{aligned}
G(t_j) &= \frac{M(\alpha)}{1-\alpha} \int_0^{t_j} f(\tau) d\tau = \frac{M(\alpha)}{\alpha} \sum_{s=0}^{j-1} \frac{f(t_{s+1}) + f(t_s)}{2} \delta_{j,s}^\alpha + H_2, \\
\delta_{j,s}^\alpha &= \exp\left(-\alpha \frac{t_j - t_{s+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_j - t_s}{1-\alpha}\right), \\
H_2 &= \frac{M(\alpha)}{1-\alpha} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \{f(\nu) - f(t_{s+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_j - \tau)\right) d\nu.
\end{aligned} \tag{5.2.5}$$

Thus, by substituting Eqs. (5.2.5) and (5.2.4) into (5.2.1), we have

$$\frac{d}{dt} U(t) = \frac{M(\alpha)}{\Delta t(\alpha)} \left[ \sum_{s=0}^j \frac{f(t_{s+1}) + f(t_s)}{2} \exp\left(-\alpha \frac{t_{j+1} - t_{s+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_{j+1} - t_s}{1-\alpha}\right) \right] + H_{\alpha,j,s}, \tag{5.2.6}$$

where

$$\begin{aligned}
H_{\alpha,j,s} &= \frac{M(\alpha)}{\Delta(\alpha)} \left\{ \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \{f(\nu) - f(t_{s+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1} - \tau)\right) d\nu \right. \\
&\quad \left. - \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \{f(\nu) - f(t_{s+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_j - \tau)\right) d\nu \right\}. \tag{5.2.7}
\end{aligned}$$

**Theorem 5.2.1** *Let  $f$  be a function not necessary differentiable on interval  $a, T$ , then the fractional derivative based on the exponential decay law of a function  $f$  of order  $\alpha$  in Riemann–Liouville sense is given as*

$${}_0^{AD} \mathcal{D}_t^\alpha \{f(t)\} = \frac{M(\alpha)}{\Delta t(\alpha)} \left[ \sum_{s=0}^j \frac{f(t_{s+1}) + f(t_s)}{2} \exp\left(-\alpha \frac{t_{j+1} - t_{s+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_{j+1} - t_s}{1-\alpha}\right) \right] + H_{\alpha,j,s}, \tag{5.2.8}$$

where

$$|H_{\alpha,j,s}| \leq M < \infty.$$

*Proof* We obtain the following from the formula  $|H_{\alpha,j,s}|$ :

$$\begin{aligned}
&\frac{M(\alpha)}{\Delta t(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \{f(\nu) - f(t_{s+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1} - \tau)\right) d\nu \\
&= \frac{M(\alpha)}{\Delta t(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \left\{ \frac{(f(\nu) - f(t_{s+1}))(\nu - t_{s+1})}{(\nu - t_{s+1})} \right\} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1} - \tau)\right) d\nu \\
&= \frac{M(\alpha)}{\Delta t(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} f'(\lambda_k)(\nu - t_{s+1}) \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1} - \tau)\right) d\nu, \quad \nu < t \leq t_{j+1}.
\end{aligned} \tag{5.2.9}$$

Thus

$$\begin{aligned} & \left| \frac{M(\alpha)}{\Delta t(1-\alpha)} \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \{f(\nu) - f(t_{s+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1}-\tau)\right) d\nu \right| \\ & \leq \frac{M(\alpha)}{1-\alpha} \max_{0 \leq t \leq t_{j+1}} |f'(t)| \sum_{s=0}^j \int_{t_s}^{t_{s+1}} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1}-\tau)\right) d\nu \quad (5.2.10) \\ & \leq \frac{M(\alpha)}{\alpha} \max_{0 \leq t \leq t_{j+1}} |f'(t)| \sum_{s=0}^j \left( \exp\left(-\alpha \frac{t_{j+1}-t_{s+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_{j+1}-t_s}{1-\alpha}\right) \right). \end{aligned}$$

Similarly,

$$\begin{aligned} & \left| \frac{M(\alpha)}{\Delta t(1-\alpha)} \sum_{s=0}^{j-1} \int_{t_s}^{t_{s+1}} \{f(\nu) - f(t_{s+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_j-\tau)\right) d\nu \right| \quad (5.2.11) \\ & \leq \frac{M(\alpha)}{\alpha} \max_{0 \leq t \leq t_{j+1}} |f'(t)| \sum_{s=0}^j \left( \exp\left(-\alpha \frac{t_j-t_{s+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_j-t_s}{1-\alpha}\right) \right). \end{aligned}$$

□

### 5.3 Numerical Approximation for Space First-Order Derivative

In the combined work by Atangana and Nieto, the Caputo–Fabrizio for order greater than 2 has been suggested and the numerical approximation was also presented in [1]. Nonetheless, we are not aware of any version in Riemann–Liouville sense, and we therefore consider the second-order space approximation of the Caputo–Fabrizio derivative in Riemann–Liouville sense here.

**Definition 5.3.1** Let  $f$  be a function (not necessarily differentiable), then the Caputo–Fabrizio fractional derivative in Riemann–Liouville sense of order bounded in  $1 < \alpha \leq 2$  is defined as

$${}^C_{FR} \mathcal{D}_x^\alpha \{f(t)\} = \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \frac{d^2}{dx^2} \int_0^x f(y) \exp\left(-\frac{\alpha^2}{(1-\alpha)}(x-y)^2\right) dy, \quad 1 < \alpha \leq 2. \quad (5.3.1)$$

In what follows, we suggest numerical approximation of this derivation, to achieve this, we let

$$U(x) = \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \frac{d^2}{dx^2} \int_0^x f(y) \exp\left(-\frac{\alpha^2}{(1-\alpha)}(x-y)^2\right) dy, \quad (5.3.2)$$

where

$${}^C_{FR} \mathcal{D}_x^\alpha \{f(t)\} = \frac{d^2 U(x)}{dx^2}.$$

By replacing the spatial second derivative with a central finite difference approximation, we have

$${}^C_{FR} \mathcal{D}_t^\alpha \{f(x)\} = \frac{d^2 U(x)}{dx^2} = \frac{U(x_{i+1}) - 2U(x_i) + U(x_{i-1}))}{2(\Delta x)^2}. \quad (5.3.3)$$

So also,

$$\begin{aligned} U(x_{j+1}) &= \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \int_0^{x_{j+1}} f(\tau) \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_{j+1} - \tau)^2 \right] d\tau, \\ &= \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \sum_{k=s}^j \int_{x_s}^{x_{s+1}} f(x_{s+1}) \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_{j+1} - \tau)^2 \right] d\tau + \mathcal{P}_1, \\ &= \frac{\alpha}{(1-\alpha)\sqrt{\pi}} f(x_{s+1}) \int_{x_s}^{x_{s+1}} \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_{j+1} - \tau)^2 \right] d\tau + \mathcal{P}_1, \\ &= \sum_{k=s}^j \frac{f(x_{s+1})}{2} \mathcal{E}_{j,k}^{\alpha,1} + \mathcal{P}_1, \end{aligned} \quad (5.3.4)$$

where

$$\mathcal{E}_{j,k}^{\alpha,1} = \operatorname{erfc} \left\{ -\alpha \frac{x_{j+1} - x_{s+1}}{1-\alpha} \right\} - \operatorname{erfc} \left\{ -\alpha \frac{x_{j+1} - x_s}{1-\alpha} \right\},$$

and

$$\mathcal{P}_1 = \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \sum_{k=s}^j \int_{x_s}^{x_{s+1}} (f(\tau) - f(x_{s+1})) \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_{j+1} - \tau)^2 \right] d\tau.$$

More so, by adopting a similar technique, we get

$$U(x_j) = \sum_{k=s}^{j-1} \frac{f(x_{s+1})}{2} \mathcal{E}_{j,k}^{\alpha,2} + \mathcal{P}_2,$$

where

$$\mathcal{E}_{j,k}^{\alpha,2} = \operatorname{erfc} \left\{ -\alpha \frac{x_j - x_{s+1}}{1-\alpha} \right\} - \operatorname{erfc} \left\{ -\alpha \frac{x_j - x_s}{1-\alpha} \right\},$$

and

$$\mathcal{P}_2 = \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \sum_{s=0}^{j-1} \int_{x_s}^{x_{s+1}} (f(\tau) - f(x_j)) \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_j - \tau)^2 \right] d\tau.$$

Also,

$$U(x_{j-1}) = \sum_{s=0}^{j-1} \frac{f(x_{s+1})}{2} \mathcal{E}_{j,k}^{\alpha,3} + \mathcal{P}_3,$$

with

$$\mathcal{E}_{j,k}^{\alpha,3} = \operatorname{erfc} \left\{ -\alpha \frac{x_{j-1} - x_{s+1}}{1-\alpha} \right\} - \operatorname{erfc} \left\{ -\alpha \frac{x_{j-1} - x_s}{1-\alpha} \right\},$$

and

$$\mathcal{P}_3 = \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \sum_{k=1}^{j-1} \int_{t_k}^{t_{k+1}} (f(\tau) - f(x_{j-1})) \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_{j-1} - \tau)^2 \right] d\tau.$$

With the above, Eq. (5.3.3) becomes

$$\begin{aligned} {}_0^{CFR} D_t^\alpha \{f(x)\} &= \frac{1}{2(\Delta x)^2} \left\{ \sum_{s=0}^j \frac{f(x_{s+1})}{2} \mathcal{E}_{j,k}^{\alpha,1} - 2 \sum_{s=0}^{j-1} \frac{f(x_{s+1})}{2} \mathcal{E}_{j,k}^{\alpha,2} + \sum_{s=0}^j \frac{f(x_{s+1})}{2} \mathcal{E}_{j,k}^{\alpha,3} \right\} + \mathcal{P}, \\ \mathcal{E}_{j,k}^{\alpha,1} &= \operatorname{erfc} \left\{ -\alpha \frac{x_{j+1} - x_{s+1}}{1-\alpha} \right\} - \operatorname{erfc} \left\{ -\alpha \frac{x_{j+1} - x_s}{1-\alpha} \right\}, \\ \mathcal{E}_{j,k}^{\alpha,2} &= \operatorname{erfc} \left\{ -\alpha \frac{x_j - x_{s+1}}{1-\alpha} \right\} - \operatorname{erfc} \left\{ -\alpha \frac{x_j - x_s}{1-\alpha} \right\}, \\ \mathcal{E}_{j,k}^{\alpha,3} &= \operatorname{erfc} \left\{ -\alpha \frac{x_{j-1} - x_{s+1}}{1-\alpha} \right\} - \operatorname{erfc} \left\{ -\alpha \frac{x_{j-1} - x_s}{1-\alpha} \right\}, \end{aligned} \quad (5.3.5)$$

$$\begin{aligned} \mathcal{P} &= \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \left\{ \sum_{s=0}^j \int_{x_s}^{x_{s+1}} (f(\tau) - f(x_{s+1})) \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_{j+1} - \tau)^2 \right] d\tau \right. \\ &\quad - 2 \sum_{s=0}^{j-1} \int_{x_s}^{x_{s+1}} (f(\tau) - f(x_j)) \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_j - \tau)^2 \right] d\tau \\ &\quad \left. + \sum_{k=1}^{j-1} \int_{t_k}^{t_{k+1}} (f(\tau) - f(x_{j-1})) \exp \left[ - \left( \frac{\alpha}{(1-\alpha)} \right)^2 (x_{j-1} - \tau)^2 \right] d\tau \right\}, \end{aligned} \quad (5.3.6)$$

the  $\operatorname{erfc}\{\cdot\}$  denotes the error function.

Conveniently, we now evaluate the first component of the reminder  $\mathcal{P}$  as

$$\begin{aligned}
|\mathcal{P}_1| &= \left| \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \sum_{s=0}^j \int_{x_s}^{x_{s+1}} (f(\tau) - f(x_{s+1})) e^{\left[-\left(\frac{\alpha}{(1-\alpha)}\right)^2 (x_{j+1}-\tau)^2\right]} d\tau \right| \\
&= \left| \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \sum_{s=0}^j \int_{x_s}^{x_{s+1}} \frac{(f(\tau) - f(x_{s+1}))(\tau - x_{s+1})}{(\tau - x_{s+1})} e^{\left[-\left(\frac{\alpha}{(1-\alpha)}\right)^2 (x_{j+1}-\tau)^2\right]} d\tau \right| \\
&= \left| \sum_{s=0}^j \int_{x_s}^{x_{s+1}} f'(y)(\tau - x_{s+1}) e^{\left[-\left(\frac{\alpha}{(1-\alpha)}\right)^2 (x_{j+1}-\tau)^2\right]} d\tau \right|, \quad \tau < y < x_{j+1} \\
&\leq \frac{\alpha \Delta x}{(1-\alpha)\sqrt{\pi}} \max_{0 \leq x \leq x_{j+1}} |f'(x)| \sum_{s=0}^j \int_{x_s}^{x_{s+1}} \exp \left[ -\left(\frac{\alpha}{(1-\alpha)}\right)^2 (x_{j+1}-\tau)^2 \right] d\tau \\
&\leq \frac{\Delta x}{2} \max_{0 \leq x \leq x_{j+1}} |f'(x)| \sum_{s=0}^j \operatorname{erfc} \left\{ -\alpha \frac{x_{j+1} - x_{s+1}}{1-\alpha} \right\} - \operatorname{erfc} \left\{ -\alpha \frac{x_{j+1} - x_s}{1-\alpha} \right\}, \\
&\Rightarrow |\mathcal{P}_1| \leq \frac{\Delta x}{2} \max_{0 \leq x \leq x_{j+1}} |f'(x)| \operatorname{erfc} \left\{ -\alpha \frac{(j+1)\Delta x}{1-\alpha} \right\}.
\end{aligned}$$

Without loss of generality, similar expressions can be obtained for the second and third terms as

$$|\mathcal{P}_2| \leq \frac{\Delta x}{2} \max_{0 \leq x \leq x_{j+1}} |f'(x)| \operatorname{erfc} \left\{ -\alpha \frac{(j)\Delta x}{1-\alpha} \right\},$$

and

$$|\mathcal{P}_3| \leq \frac{\Delta x}{2} \max_{0 \leq x \leq x_{j+1}} |f'(x)| \operatorname{erfc} \left\{ -\alpha \frac{(j-1)\Delta x}{1-\alpha} \right\}.$$

**Definition 5.3.2** Let  $f(x)$  be a function in  $C^2[a, b]$  and let the order of the fractional derivative be  $0 < \alpha \leq 1$ , then the first-order approximation of the Caputo–Fabrizio derivative at a point  $t_n$  is given by [1]

$${}_0^{CF} \mathcal{D}_t^\alpha (f(t_n)) = \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \left( \frac{f^{j+1} - f^j}{k} \right) \mu_{j,k} + \frac{M(\alpha)}{\alpha} \sum_{j=1}^n \mu_{j,k} \mathcal{O}(k), \quad (5.3.7)$$

where

$$\mu_{j,k} = -\exp \left[ -\alpha \frac{k}{k-\alpha} (n-j+1) \right] + \exp \left[ -\alpha \frac{k}{1-\alpha} (n-j) \right].$$

**Definition 5.3.3** Let  $f(x, t)$  be a function in  $C^2([a, b] \times [0, T])$  and let the order of the fractional derivative be  $0 < \alpha \leq 1$ , then the first-order approximation of the Caputo–Fabrizio derivative at a point  $(x_m, t_n)$  is given by [1]

$$\begin{aligned}
{}_0^{CF}\mathcal{D}_x^\alpha(f(x_m, t_k)) &= \frac{M(\alpha)}{(1-\alpha)} \sum_{s=1}^m \left\{ \frac{(f_{i+1}^{k+1} - f_{i-1}^{k+1}) - (f_{i+1}^k - f_{i-1}^k)(1-\alpha)\sqrt{\pi}}{4i} \frac{(1-\alpha)\sqrt{\pi}}{2\alpha} \right. \\
&\quad \left. \left\{ \operatorname{erf}\left[(m-s)\frac{\alpha i}{1-\alpha}\right] - \operatorname{erf}\left[(m-s+1)\frac{\alpha i}{1-\alpha}\right] \right\} \right\} \\
&\quad + \mathcal{O}(i) \frac{(1-\alpha)}{2\alpha} \sum_{s=1}^m \left\{ \operatorname{erf}\left[(m-s)\frac{\alpha i}{1-\alpha}\right] - \operatorname{erf}\left[(m-s+1)\frac{\alpha i}{1-\alpha}\right] \right\}.
\end{aligned} \tag{5.3.8}$$

## 5.4 Numerical Approximation for Space Second-Order Derivative

**Theorem 5.4.1** *Let  $f(x, t)$  be twice differentiable on both  $x$ - and  $t$ -directions, then the second derivative approximation of the Caputo–Fabrizio fractional derivative of function  $f(x, t)$  is defined as*

$$\begin{aligned}
{}_0^{CF}\mathcal{D}_t^\alpha(f(x_j, t)) &= \frac{1}{2} \sum_{k=1}^j \left\{ \frac{(f_{i+1}^{k+1} - 2f_i^{k+1} + f_{i-1}^{k+1}) + (f_{i+1}^k - 2f_i^k + f_{i-1}^k)}{2(\Delta x)^2} \right\} \\
&\quad \times \left\{ \operatorname{erf}\left[\frac{\alpha}{1-\alpha}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\alpha}{1-\alpha}(x_j - x_k)\right] \right\} + \mathcal{O}((\Delta x)^2).
\end{aligned} \tag{5.4.1}$$

*Proof* The corresponding second order of the new fractional derivative is given by

$${}_0^{CF}\mathcal{D}_x^\alpha(f(x, t)) = \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \int_0^x \frac{\partial^2 f(r, t)}{\partial r^2} \exp\left[-\frac{\alpha^2(x-r)^2}{(1-\alpha)^2}\right] dr. \tag{5.4.2}$$

However, for any given  $x_j$ , we obtain

$${}_0^{CF}\mathcal{D}_x^\alpha(f(x_j, t)) = \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \sum_{i=1}^j \int_{x_k}^{x_{k+1}} \frac{\partial^2 f(r, t)}{\partial r^2} \exp\left[-\frac{\alpha^2(x_j - r)^2}{(1-\alpha)^2}\right] dr. \tag{5.4.3}$$

By applying the Crank–Nicholson scheme to the usual second-order derivative, the scheme is reformulated to

$$\begin{aligned}
{}_0^{CF}\mathcal{D}_x^\alpha(f(x_j, t)) &= \frac{\alpha}{(1-\alpha)\sqrt{\pi}} \times \\
&\quad \sum_{i=1}^j \left\{ \frac{(f_{i+1}^{k+1} - 2f_i^{k+1} + f_{i-1}^{k+1}) + (f_{i+1}^k - 2f_i^k + f_{i-1}^k)}{2(\Delta x)^2} + \mathcal{O}((\Delta x)^2) \right\} \\
&\quad \left[ \int_{x_k}^{x_{k+1}} \exp\left[-\frac{\alpha^2(x_j - r)^2}{(1-\alpha)^2}\right] dr \right],
\end{aligned} \tag{5.4.4}$$

where  $f(x_j, t_i) = f_i^j$ .

Nevertheless, we evaluate the integral in the right-hand side of the above equation as

$$\begin{aligned} & \int_{x_k}^{x_{k+1}} \exp\left[-\frac{\alpha^2(x_j - r)^2}{(1 - \alpha)^2}\right] dr \\ &= \frac{(1 - \alpha)\sqrt{\pi}}{2\alpha} \left\{ \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_k)\right] \right\}. \end{aligned} \quad (5.4.5)$$

As a result, Eq. (5.4.4) becomes

$$\begin{aligned} {}_0^{CF}\mathcal{D}_x^\alpha(f(x_j, t)) &= \frac{1}{2} \sum_{i=1}^j \left\{ \frac{(f_{i+1}^{k+1} - 2f_i^{k+1} + f_{i-1}^{k+1}) + (f_{i+1}^k - 2f_i^k + f_{i-1}^k)}{2(\Delta x)^2} + \mathcal{O}((\Delta x)^2) \right\} \\ &\quad \times \left\{ \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_k)\right] \right\}. \end{aligned} \quad (5.4.6)$$

The above equation can be rewritten as follows:

$$\begin{aligned} {}_0^{CF}\mathcal{D}_x^\alpha(f(x_j, t)) &= \frac{1}{2} \sum_{i=1}^j \left\{ \frac{(f_{i+1}^{k+1} - 2f_i^{k+1} + f_{i-1}^{k+1}) + (f_{i+1}^k - 2f_i^k + f_{i-1}^k)}{2(\Delta x)^2} \right\} \\ &\quad \times \left\{ \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_k)\right] \right\} \\ &\quad + \sum_{i=1}^j \left\{ \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_k)\right] \right\} + \mathcal{O}((\Delta x)^2). \end{aligned} \quad (5.4.7)$$

Take note that

$$\sum_{i=1}^j \left\{ \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_k)\right] \right\} = \operatorname{erf}\left[\frac{-j\alpha}{1 - \alpha} \Delta x\right].$$

By adopting the Abramowitz and Stegun series approximation of the error function, Eq. (5.4.7) reduces to

$$\begin{aligned} {}_0^{CF}\mathcal{D}_x^\alpha(f(x_j, t)) &= \frac{1}{2} \sum_{i=1}^j \left\{ \frac{(f_{i+1}^{k+1} - 2f_i^{k+1} + f_{i-1}^{k+1}) + (f_{i+1}^k - 2f_i^k + f_{i-1}^k)}{2(\Delta x)^2} \right\} \\ &\quad \times \left\{ \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\alpha}{1 - \alpha}(x_j - x_k)\right] \right\} + \mathcal{O}((\Delta x)^2). \end{aligned} \quad (5.4.8)$$

□

### 5.4.1 Three-Step Adams–Bashforth Scheme with Caputo–Fabrizio Fractional Derivative

Here, we consider the following general fractional differential equation with fading memory included via the Caputo–Fabrizio fractional derivative. That is,

$${}_0^C D_t^\alpha u(t) = f(t, u(t)) \quad (5.4.9)$$

or

$$\frac{M(\alpha)}{1-\alpha} \int_0^t u'(\xi) \exp\left[-\frac{\alpha}{1-\alpha}(t-\xi)\right] d\xi = f(t, u(t)). \quad (5.4.10)$$

Using the fundamental theorem of calculus, we convert the above to

$$u(t) - u(0) = \frac{1-\alpha}{M(\alpha)} f(t, u(t)) + \frac{\alpha}{M(\alpha)} \int_0^t f(\xi, u(\xi)) d\xi \quad (5.4.11)$$

so that

$$u(t_{n+1}) - u(0) = \frac{1-\alpha}{M(\alpha)} f(t_n, u(t_n)) + \frac{\alpha}{M(\alpha)} \int_0^{t_{n+1}} f(t, u(t)) dt \quad (5.4.12)$$

and

$$u(t_n) - u(0) = \frac{1-\alpha}{M(\alpha)} f(t_{n-1}, u(t_{n-1})) + \frac{\alpha}{M(\alpha)} \int_0^{t_n} f(t, u(t)) dt. \quad (5.4.13)$$

On removing (5.4.13) from (5.4.12), we obtain

$$u(t_{n+1}) - u(t_n) = \frac{1-\alpha}{M(\alpha)} \{f(t_n, u_n) - f(t_{n-1}, u_{n-1})\} + \frac{\alpha}{M(\alpha)} \int_{t_n}^{t_{n+1}} f(t, u(t)) dt, \quad (5.4.14)$$

where

$$\begin{aligned} \int_{t_n}^{t_{n+1}} f(t, u(t)) dt &= \int_{t_n}^{t_{n+1}} \left\{ \frac{f(t_n, u_n)}{h} (t - t_n) - \frac{f(t_{n-1}, u_{n-1})}{h} (t - t_{n-1}) \right. \\ &\quad \left. + \frac{f(t_{n-2}, u_{n-2})}{h} (t - t_n) \right\} dt \\ &= \frac{23h}{12} f(t_n, u_n) - \frac{16h}{12} f(t_{n-1}, u_{n-1}) + \frac{5h}{12} f(t_{n-2}, u_{n-2}). \end{aligned} \quad (5.4.15)$$

Thus,

$$\begin{aligned} u(t_{n+1}) - u(t_n) &= \frac{1-\alpha}{M(\alpha)} [f(t_n, u_n) - f(t_{n-1}, u_{n-1})] \\ &\quad + \frac{\alpha h}{12M(\alpha)} [23f(t_n, u_n) - 16f(t_{n-1}, u_{n-1}) + 5f(t_{n-2}, u_{n-2})] \end{aligned}$$

which implies that

$$u(t_{n+1}) - u(t_n) = \left( \frac{1-\alpha}{M(\alpha)} + \frac{23\alpha h}{12M(\alpha)} \right) f(t_n, u_n) - \left( \frac{1-\alpha}{M(\alpha)} + \frac{16\alpha h}{12M(\alpha)} \right) f(t_{n-1}, u_{n-1}) + \frac{5\alpha h}{12M(\alpha)} f(t_{n-2}, u_{n-2}). \quad (5.4.16)$$

Hence,

$$u_{n+1} = u_n + \left( \frac{1-\alpha}{M(\alpha)} + \frac{23\alpha h}{12M(\alpha)} \right) f(t_n, u_n) - \left( \frac{1-\alpha}{M(\alpha)} + \frac{16\alpha h}{12M(\alpha)} \right) f(t_{n-1}, u_{n-1}) + \frac{5\alpha h}{12M(\alpha)} f(t_{n-2}, u_{n-2}) + R_n^\alpha(t) \quad (5.4.17)$$

which is the three-step Adams–Bashforth scheme for the Caputo–Fabrizio fractional derivative, where

$$\begin{aligned} R_n^\alpha(t) &= \frac{\alpha}{M(\alpha)} \int_0^t \frac{3}{8} f^{(4)}(\xi) h^3 d\xi \\ \|R_n^\alpha(t)\|_\infty &= \frac{\alpha}{M(\alpha)} \left\| \int_0^t \frac{3}{8} f^{(4)}(\xi) h^3 \right\|_\infty d\xi \\ &\leq \frac{3\alpha h^3}{8M(\alpha)} \int_0^t \|f^{(4)}(\xi)\|_\infty d\xi \\ &\leq \frac{3\alpha h^3}{8M(\alpha)} T_{max}(\beta), \end{aligned} \quad (5.4.18)$$

where

$$\beta = \max_{\xi \in [0, t]} \|f^{(4)}(\xi)\|_\infty.$$

*Remark 5.4.2* Clearly, with  $\alpha = 1$  in (5.4.17), we recover the classical Adams–Bashforth three-step explicit scheme

$$u_{n+1} = u_n + \frac{h}{12} [23f(t_n, u_n) - 16f(t_{n-1}, u_{n-1}) + 5f(t_{n-2}, u_{n-2})]. \quad (5.4.19)$$

## 5.4.2 Stability Analysis

Here, we examine the stability analysis of the three-step fractional Adams–Bashforth scheme (5.4.17), by considering equation

$${}^C D_t^\alpha u(t) = u(t), \quad (5.4.20)$$

where  ${}_0^C \mathcal{D}_t^\alpha$  is the Caputo–Fabrizio derivative of order  $\alpha$ . Recall that

$$\begin{aligned} u_{n+1} &= u_n + \underbrace{\left( \frac{1-\alpha}{M(\alpha)} + \frac{23\alpha h}{12M(\alpha)} \right)}_A f(t_n, u_n) - \underbrace{\left( \frac{1-\alpha}{M(\alpha)} + \frac{16\alpha h}{12M(\alpha)} \right)}_B f(t_{n-1}, u_{n-1}) \\ &\quad + \underbrace{\frac{5\alpha h}{12M(\alpha)}}_C f(t_{n-2}, u_{n-2}) \\ &= u_n + Af(t_n, u_n) - Bf(t_{n-1}, u_{n-1}) + Cf(t_{n-2}, u_{n-2}). \end{aligned} \quad (5.4.21)$$

By using (5.4.20), the above equation becomes

$$u_{n+1} = (1 + A)u_n - Bu_{n-1} + Cu_{n-2}. \quad (5.4.22)$$

Next, we adopt the von Neumann stability analysis for the terms in above equation as

$$\begin{aligned} u_{n+1} &= \hat{u}_{n+1} e^{(n+1)i\Delta t}, \\ u_n &= \hat{u}_n e^{ni\Delta t}, \\ u_{n-1} &= \hat{u}_{n-1} e^{(n-1)i\Delta t}, \\ u_{n-2} &= \hat{u}_{n-2} e^{(n-2)i\Delta t}. \end{aligned} \quad (5.4.23)$$

So that

$$\bar{u}_{n+1} e^{(n+1)i\Delta t} = (1 + A)\bar{u}_n e^{ni\Delta t} - B\bar{u}_{n-1} e^{(n-1)i\Delta t} + C\bar{u}_{n-2} e^{(n-2)i\Delta t}, \quad (5.4.24)$$

which reduces to

$$\bar{u}_{n+1} e^{i\Delta t} = (1 + A)\bar{u}_n - B\bar{u}_{n-1} e^{-i\Delta t} + C\bar{u}_{n-2} e^{-2i\Delta t}. \quad (5.4.25)$$

We apply a recursive formula:

when  $n = 0$ ,

$$\bar{u}_1 e^{i\Delta t} = (1 + A)\bar{u}_0. \quad (5.4.26)$$

By taking the norms of both sides, we have

$$\|\bar{u}_1 e^{i\Delta t}\| = \|(1 + A)\hat{u}_0\|$$

$$\implies \|\hat{u}_1\| = (1 + A)\|\hat{u}_0\|.$$

If

$$h \leq 0.55 \quad \text{and} \quad \alpha > \frac{1}{1 - 1.9167h},$$

then, we assume that

$$\forall n \geq |\hat{u}_n| < |\hat{u}_0|,$$

so that

$$\begin{aligned} |\hat{u}_{n+1}| &\leq (1 + A)|\hat{u}_n||e^{-i\Delta t}| - B|\hat{u}_{n-1}||e^{-2i\Delta t}| + C|\hat{u}_{n-2}||e^{-3i\Delta t}| \\ &< (1 + A)|\hat{u}_n| - B|\hat{u}_{n-1}| + C|\hat{u}_{n-2}|. \end{aligned} \quad (5.4.27)$$

By hypothesis, we have

$$\begin{aligned} |\hat{u}_{n+1}| &< (1 + A)|\hat{u}_0| - B|\hat{u}_0| + C|\hat{u}_0| \\ &< (1 + A - B + C)|\hat{u}_0| \\ &< (1 + A - B + C) < 1. \end{aligned} \quad (5.4.28)$$

Hence, the three-step Adams–Bashforth scheme with the Caputo derivative is conditionally stable when applied to equation of the form (5.4.20).

### 5.4.3 Applications

Let us consider

$${}_0^{CF} \mathcal{D}_t^\alpha u(t) = u(t) + g(t), \quad (5.4.29)$$

where  $g(t)$  is a known function. By applying the Caputo–Fabrizio derivative, we obtain

$$\frac{M(\alpha)}{1 - \alpha} \int_0^t \frac{du}{d\xi}(\xi) \exp\left[-\frac{\alpha(t - \xi)}{1 - \alpha}\right] d\xi = u(t) + g(t). \quad (5.4.30)$$

By applying the convolution theorem, the above equation becomes

$$\frac{M(\alpha)}{1 - \alpha} \frac{du}{dt} \exp\left[-\frac{\alpha t}{1 - \alpha}\right] = u(t) + g(t). \quad (5.4.31)$$

Next, we take the Laplace transform of both sides as

$$\mathcal{L} \left\{ \frac{M(\alpha)}{1 - \alpha} \frac{du}{dt} \exp\left[-\frac{\alpha t}{1 - \alpha}\right] \right\} = \mathcal{L}\{u(t)\} + \mathcal{L}g(t) \quad (5.4.32)$$

which implies

$$\frac{M(\alpha)}{1 - \alpha} \mathcal{L} \left( \frac{du}{dt} \right) \mathcal{L} \left\{ \exp\left[-\frac{\alpha t}{1 - \alpha}\right] \right\} = \tilde{u}(p) + \tilde{g}(p). \quad (5.4.33)$$

That is,

$$\begin{aligned} \frac{M(\alpha)}{1-\alpha} [p\tilde{u}(p) - u(0)] \cdot \frac{1}{p + \frac{\alpha}{1-\alpha}} &= \tilde{u}(p) + \tilde{g}(p) \\ \tilde{u}(p) \left[ \frac{M(\alpha)}{1-\alpha} \frac{p}{p + \frac{\alpha}{1-\alpha}} - 1 \right] &= \frac{M(\alpha)}{1-\alpha} \cdot \frac{u(0)}{p + \frac{\alpha}{1-\alpha}} + \tilde{g}(p) \\ \tilde{u}(p) \left[ \frac{p \left( \frac{M(\alpha)}{1-\alpha} - 1 \right) - \frac{\alpha}{1-\alpha}}{p + \frac{\alpha}{1-\alpha}} \right] &= \frac{M(\alpha)}{1-\alpha} \cdot \frac{u(0)}{p + \frac{\alpha}{1-\alpha}} + \tilde{g}(p). \end{aligned}$$

On rearranging, we obtain

$$\tilde{u}(p) = \frac{M(\alpha)}{1-\alpha} \cdot \frac{u(0)}{p + \frac{\alpha}{1-\alpha}} \left( \frac{p + \frac{\alpha}{1-\alpha}}{p \left[ \frac{M(\alpha)}{1-\alpha} - 1 \right] - \frac{\alpha}{1-\alpha}} \right) + \frac{\tilde{g}(p) \left( p + \frac{\alpha}{1-\alpha} \right)}{p \left[ \frac{M(\alpha)}{1-\alpha} - 1 \right] - \frac{\alpha}{1-\alpha}}, \quad (5.4.34)$$

which simplifies into

$$\tilde{u}(p) = \underbrace{\frac{M(\alpha)}{1-\alpha} \left( \frac{u(0)}{p \left[ \frac{M(\alpha)}{1-\alpha} - 1 \right] - \frac{\alpha}{1-\alpha}} \right)}_A + \underbrace{\frac{\tilde{g}(p) \left( p + \frac{\alpha}{1-\alpha} \right)}{p \left[ \frac{M(\alpha)}{1-\alpha} - 1 \right] - \frac{\alpha}{1-\alpha}}}_B. \quad (5.4.35)$$

Starting with  $A$ , we find the inverse Laplace transform as

$$\begin{aligned} u(t) = \mathcal{L}\{\tilde{u}(p)\} &= \frac{M(\alpha)}{1-\alpha} \cdot \frac{u(0)}{\frac{M(\alpha)}{1-\alpha} - 1} \mathcal{L} \left\{ \frac{1}{p - \frac{\alpha}{M(\alpha) + \alpha - 1}} \right\} \\ &= \left( \frac{M(\alpha)}{M(\alpha) + \alpha - 1} \right) u(0) \left[ \mathcal{L} \left\{ \frac{1}{p - \frac{\alpha}{M(\alpha) + \alpha - 1}} \right\} \right] \end{aligned} \quad (5.4.36)$$

so that

$$u_1(t) = \frac{u(0)M(\alpha)}{M(\alpha) + \alpha - 1} \exp \left[ \frac{\alpha t}{M(\alpha) + \alpha - 1} \right]. \quad (5.4.37)$$

Similarly for the part  $B$ , we find the inverse Laplace transform as

$$\begin{aligned}
 u(t) = \mathcal{L}\{\tilde{u}(p)\} &= \frac{1}{\frac{M(\alpha)}{1-\alpha} - 1} \left[ \frac{\tilde{g}(p) \cdot p}{p - \frac{\alpha}{\frac{1-\alpha}{M(\alpha)} - 1}} + \frac{\tilde{g}(p) \frac{\alpha}{1-\alpha}}{p - \frac{\alpha}{\frac{1-\alpha}{M(\alpha)} - 1}} \right] \\
 &= \frac{1-\alpha}{M(\alpha) + \alpha - 1} \left[ \frac{\tilde{g}(p) \cdot p}{p - \frac{1}{M(\alpha) + \alpha - 1}} + \frac{\tilde{g}(p) \frac{\alpha}{1-\alpha}}{p - \frac{1}{M(\alpha) + \alpha - 1}} \right] \\
 &= \frac{1-\alpha}{M(\alpha) + \alpha - 1} \left[ \tilde{g}(p) \left( \frac{p - \frac{1}{M(\alpha) + \alpha - 1} + \frac{1}{M(\alpha) + \alpha - 1}}{p - \frac{1}{M(\alpha) + \alpha - 1}} \right) + \frac{\tilde{g}(p) \frac{\alpha}{1-\alpha}}{p - \frac{1}{M(\alpha) + \alpha - 1}} \right] \\
 &= \frac{1-\alpha}{M(\alpha) + \alpha - 1} \left[ \tilde{g}(p) + \frac{\tilde{g}(p) \left( \frac{\alpha}{1-\alpha} + \frac{1}{M(\alpha) + \alpha - 1} \right)}{p - \frac{1}{M(\alpha) + \alpha - 1}} \right]
 \end{aligned}
 \tag{5.4.38}$$

which by inverse Laplace transform, we have

$$\begin{aligned}
 u_2(t) &= \left( \frac{1-\alpha}{M(\alpha) + \alpha - 1} \right) g(t) + \left( \frac{1-\alpha}{M(\alpha) + \alpha - 1} \right) \left( \frac{\alpha}{1-\alpha} + \frac{1}{M(\alpha) + \alpha - 1} \right) \\
 &\quad \times \int_0^t g(\xi) \exp \left[ \frac{t-\xi}{M(\alpha) + \alpha - 1} \right] d\xi.
 \end{aligned}
 \tag{5.4.39}$$

Finally, the exact solution for (5.4.29) is obtained as

$$\begin{aligned}
 u(t) &= \frac{u(0)M(\alpha)}{M(\alpha) + \alpha - 1} \exp \left[ \frac{\alpha t}{M(\alpha) + \alpha - 1} \right] + \left( \frac{1-\alpha}{M(\alpha) + \alpha - 1} \right) g(t) \\
 &\quad + \left( \frac{1-\alpha}{M(\alpha) + \alpha - 1} \right) \left( \frac{\alpha}{1-\alpha} + \frac{1}{M(\alpha) + \alpha - 1} \right) \int_0^t g(\xi) \exp \left[ \frac{t-\xi}{M(\alpha) + \alpha - 1} \right] d\xi.
 \end{aligned}
 \tag{5.4.40}$$

## References

1. A. Atangana, J.J. Nieto, Numerical solution for the model of RLC circuit via the fractional derivative without singular kernel. *Adv. Mech. Eng.* **7**, 1–6 (2015)
2. A. Atangana, R.T. Alqahtani, Numerical approximation of the space-time Caputo-Fabrizio fractional derivative and application to groundwater pollution equation. *Adv. Differ. Equ.* **2016**(1), 1–13 (2016)
3. M. Caputo, M. Fabrizio, A new definition of fractional derivative without singular kernel. *Prog. Fract. Differ. Appl.* **1**, 73–85 (2015)
4. M. Caputo, M. Fabrizio, Applications of new time and spatial fractional derivatives with exponential kernels. *Prog. Fract. Differ. Appl.* **2**, 1–11 (2016)
5. E.F.D. Goufo, A. Atangana, Analytical and numerical schemes for a derivative with filtering property and no singular kernel with applications to diffusion. *Eur. Phys. J. Plus* **131**, 269 (2016). <https://doi.org/10.1140/epjp/i2016-16269-1>

# Chapter 6

## Numerical Approximation of Atangana–Baleanu Differentiation



Recently, a new contribution was made in the field of fractional calculus where new differential operators are with non-singular and non-local kernel. The new kernel introduced is the well-known generalized Mittag–Leffler function and the properties of this function enable the new operators to have some interesting properties that are observed in real-world situation, for instance, the crossover of the mean square displacement and scaling variant. The fractional differential operators have been applied intensively in several fields since were suggested in 2016. Due to their wider applicability, these operators gave birth to fractional differential equations with no artificial singularities as in the case of Riemann–Caputo derivatives, but with non-local behaviour. We have also seen an interest of these operators in the field of numerical analysis. Thus, to accommodate readers interesting in applying these derivatives to numerical analysis, we present in this chapter some numerical scheme in connection with the Atangana–Baleanu fractional differential operators.

### 6.1 Atangana–Baleanu Fractional Derivative in Caputo Sense

Let us examine the following fractional differential equation:

$${}^{ABC}D_t^\alpha u(t) = f(t, u(t)). \quad (6.1.1)$$

Again, we apply the fundamental theorem of calculus to have

$$u(t) - u(0) = \frac{1 - \alpha}{ABC(\alpha)} f(t, u(t)) + \frac{\alpha}{ABC(\alpha)\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} f(\tau, u(\tau)) d\tau. \quad (6.1.2)$$

At  $t_{n+1}$ , we have

$$u(t_{n+1}) - u(0) = \frac{1 - \alpha}{ABC(\alpha)} f(t_n, u_n) + \frac{\alpha}{ABC(\alpha)\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - \tau)^{\alpha-1} f(t, u(t)) dt$$

and at  $t_n$  we have

$$u(t_n) - u(0) = \frac{1 - \alpha}{ABC(\alpha)} f(t_{n-1}, u_{n-1}) + \frac{\alpha}{ABC(\alpha)\Gamma(\alpha)} \int_0^{t_n} (t_n - \tau)^{\alpha-1} f(t, u(t)) dt$$

which on subtraction yields

$$\begin{aligned} u(t_{n+1}) - u(t_n) &= \frac{1 - \alpha}{ABC(\alpha)} \{f(t_n, u_n) - f(t_{n-1}, u_{n-1})\} \\ &\quad + \frac{\alpha}{ABC(\alpha)\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} \\ &\quad \times f(t, u(t)) dt - \frac{\alpha}{ABC(\alpha)\Gamma(\alpha)} \int_0^{t_n} (t_n - t)^{\alpha-1} f(t, u(t)) dt. \end{aligned} \quad (6.1.3)$$

Therefore,

$$u(t_{n+1}) - u(t_n) = \frac{1 - \alpha}{ABC(\alpha)} \{f(t_n, u_n) - f(t_{n-1}, u_{n-1})\} + A_{\alpha,1} - A_{\alpha,2}.$$

Without loss of generality, we consider

$$A_{\alpha,1} = \frac{\alpha}{ABC(\alpha)\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} f(t, u(t)) dt.$$

Again we consider the approximation

$$p(t) = \frac{t - t_{n-1}}{t_n - t_{n-1}} f(t_n, u_n) + \frac{t - t_n}{t_{n-1} - t_n} f(t_{n-1}, u_{n-1}), \quad (6.1.4)$$

thus

$$\begin{aligned} A_{\alpha,1} &= \frac{\alpha}{ABC(\alpha)\Gamma(\alpha)} \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} \left\{ \frac{t - t_{n-1}}{h} f(t_n, u_n) - \frac{t - t_n}{h} f(t_n, u_n) \right\} \\ &= \frac{\alpha f(t_n, u_n)}{ABC(\alpha)\Gamma(\alpha)h} \left\{ \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} f(t - t_{n-1}) \right\} dt \\ &\quad - \frac{\alpha f(t_{n-1}, u_{n-1})}{ABC(\alpha)\Gamma(\alpha)h} \left\{ \int_0^{t_{n+1}} (t_{n+1} - t)^{\alpha-1} f(t - t_{n-1}) \right\} dt \quad (6.1.5) \\ &= \frac{\alpha f(t_n, u_n)}{ABC(\alpha)\Gamma(\alpha)h} \left[ \frac{2ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right] - \frac{\alpha f(t_{n-1}, u_{n-1})}{ABC(\alpha)\Gamma(\alpha)h} \left[ \frac{ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right]. \end{aligned}$$

Similarly, we obtain

$$A_{\alpha,2} = \frac{\alpha f(t_n, u_n)}{ABC(\alpha)\Gamma(\alpha)h} \left\{ \frac{ht_n^\alpha}{\alpha} - \frac{t_n^{\alpha+1}}{\alpha+1} \right\} - \frac{f(t_{n-1}, u_{n-1})}{ABC(\alpha)\Gamma(\alpha)h} \quad (6.1.6)$$

thus

$$\begin{aligned} & u(t_{n+1}) - u(t_n) \\ &= \frac{1-\alpha}{ABC(\alpha)} \{f(t_n, u_n) - f(t_{n-1}, u_{n-1})\} + \frac{\alpha f(t_n, u_n)}{ABC(\alpha)\Gamma(\alpha)h} \left\{ \frac{2ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right\} \\ & - \frac{\alpha f(t_{n-1}, u_{n-1})}{ABC(\alpha)\Gamma(\alpha)h} \left\{ \frac{ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right\} - \frac{\alpha f(t_n, u_n)}{ABC(\alpha)\Gamma(\alpha)h} \left\{ \frac{ht_n^\alpha}{\alpha} - \frac{t_n^{\alpha+1}}{\alpha+1} \right\} \\ & + \frac{f(t_{n-1}, u_{n-1})}{ABC(\alpha)\Gamma(\alpha)} t_n^{\alpha+1}. \end{aligned} \quad (6.1.7)$$

$$\begin{aligned} u_{(n+1)} &= u(t_n) + f(t_n, u_n) \left\{ \frac{1-\alpha}{AB(\alpha)} + \frac{\alpha}{ABC(\alpha)h} \left[ \frac{2ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} \right] \right. \\ & \quad \left. - \frac{\alpha}{AB(\alpha)\Gamma(\alpha)h} \left[ \frac{ht_n^\alpha}{\alpha} - \frac{t_n^{\alpha+1}}{\alpha+1} \right] \right\} + f(t_{n-1}, u_{n-1}) \\ & \quad \times \left\{ \frac{\alpha-1}{AB(\alpha)} - \frac{\alpha}{h\Gamma(\alpha)AB(\alpha)} \left[ \frac{ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha+1} + \frac{t^{\alpha+1}}{h\Gamma(\alpha)AB(\alpha)} \right] \right\}. \end{aligned} \quad (6.1.8)$$

This equation is known as the two-step Adams–Bashforth scheme for Atangana–Baleanu fractional derivative in the sense of Caputo.

Further, we simplify the last equation by putting  $t_n = nh$  and  $t_{n+1} = (n+1)h$ , and collect the resulting equation in powers of  $h$  to yield

$$\begin{aligned} u_{n+1} &= u_n + f(t_n, u_n) \left\{ \frac{1-\alpha}{AB(\alpha)} - \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} h^\alpha \left[ \frac{2(n+1)^\alpha}{\alpha} - \frac{(n+1)^{\alpha+1}}{\alpha+1} \right] \right. \\ & \quad \left. - \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} h^\alpha \left[ \frac{n^\alpha}{\alpha} - \frac{n^{\alpha+1}}{\alpha+1} \right] \right\} + f(t_{n-1}, u_{n-1}) \\ & \quad \times \left\{ \frac{\alpha-1}{AB(\alpha)} - \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} h^\alpha \left[ \frac{(n+1)^\alpha}{\alpha} - \frac{(n+1)^{\alpha+1}}{\alpha+1} + \frac{n^{\alpha+1}}{AB(\alpha)\Gamma(\alpha)h} \right] \right\}. \end{aligned} \quad (6.1.9)$$

In the following, we briefly outline the convergence and stability results previously obtained in [1].

**Theorem 6.1.1** (Convergence result [1]) *Let  $u(t)$  be a solution of*

$${}_0^{ABC} \mathcal{D}_t^\alpha u(t) = f(t, u(t))$$

*with  $f$  being continuous and bounded; the numerical solution of  $u(t)$  is given as*

$$\begin{aligned}
 u_{n+1} = u_n + f(t_n, u_n) & \left\{ \frac{1 - \alpha}{AB(\alpha)} + \frac{\alpha}{AB(\alpha)h} \left[ \frac{2ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha + 1} \right] \right. \\
 & \left. - \frac{\alpha}{AB(\alpha)\Gamma(\alpha)h} \left[ \frac{ht_n^\alpha}{\alpha} - \frac{t_n^{\alpha+1}}{\alpha + 1} \right] \right\} + f(t_{n-1}, u_{n-1}) \\
 & \times \left\{ \frac{\alpha - 1}{AB(\alpha)} - \frac{\alpha}{h\Gamma(\alpha)AB(\alpha)} \left[ \frac{ht_{n+1}^\alpha}{\alpha} - \frac{t_{n+1}^{\alpha+1}}{\alpha + 1} + \frac{t^{\alpha+1}}{h\Gamma(\alpha)AB(\alpha)} \right] \right\} + R_\alpha,
 \end{aligned}$$

where  $\|R_\alpha\|_\infty < M$ .

**Theorem 6.1.2** (Condition for stability [1]) *If  $f$  satisfies a Lipschitz condition, then the required stability condition for Adams–Bashforth method when applied to approximate the Atangana–Baleanu derivative of fractional order in Caputo sense is achieved if*

$$\|f(t_n, u_n) - f(t_{n-1}, u_{n-1})\|_\infty \rightarrow 0$$

as  $n \rightarrow \infty$ .

## 6.2 Uniqueness and Existence of Solution via Chaotic Process

In this section, we choose a chaotic system to test the existence and uniqueness of the new Adams–Bashforth method with the Atangana–Baleanu derivative in the sense of Caputo. To start with, we consider the general two-component system:

$$\begin{aligned}
 {}_0^{ABC} \mathcal{D}_t^\alpha x(t) &= f(x, y, t), \\
 {}_0^{ABC} \mathcal{D}_t^\alpha y(t) &= g(x, y, t).
 \end{aligned}
 \tag{6.2.1}$$

By adopting the fundamental calculus theorem along  $x$  and  $y$  components, we have

$$\begin{aligned}
 x(t) - x(0) &= \frac{1 - \alpha}{AB(\alpha)} f(x, y, t) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} f(x, y, \tau) d\tau \\
 y(t) - y(0) &= \frac{1 - \alpha}{AB(\alpha)} g(x, y, t) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} g(x, y, \tau) d\tau.
 \end{aligned}
 \tag{6.2.2}$$

Next, we require to create a compact  $G_{a,b}$ , which means

$$G_{a,b} = I_a(t_0) \times \mathcal{B}_b(\xi),
 \tag{6.2.3}$$

where

$$\xi = \min\{x_0, x_0\}$$

and

$$I_a(t_0) = [t_0 - a, t_0 + a], \quad \mathcal{B}_0(\xi) = [\xi - b, \xi + b].$$

Let

$$M = \max_{G_{a,b}} \left\{ \sup_{G_{a,b}} \|f\|, \sup_{G_{a,b}} \|g\| \right\}.$$

By applying the infinite norm, we obtain

$$\|\Phi\|_\infty = \sup_{t \in I_a} |\Phi(t)|.$$

Next, we create a function, say

$$\Gamma : G_{a,b} \rightarrow G_{a,b}$$

so that

$$\begin{aligned} \Gamma x(t) &= x_0 + \frac{1-\alpha}{AB(\alpha)} f(x, y, t) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t f(x, y, t)(t-\tau)^{\alpha-1} d\tau \\ \Gamma y(t) &= y_0 + \frac{1-\alpha}{AB(\alpha)} g(x, y, t) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t g(x, y, t)(t-\tau)^{\alpha-1} d\tau. \end{aligned} \quad (6.2.4)$$

Next, we prove that the new fractional operator is well defined by evaluating the condition for which

$$\begin{aligned} \|\Gamma_1 x(t) - x_0\|_\infty &< b, \\ \|\Gamma_2 y(t) - y_0\|_\infty &< b. \end{aligned} \quad (6.2.5)$$

So, beginning with the  $x$ -component, we get

$$\begin{aligned} \|\Gamma_1 x(t) - x_0\|_\infty &= \left\| \frac{1-\alpha}{AB(\alpha)} f(x, y, t) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t f(x, y, t)(t-\tau)^{\alpha-1} d\tau \right\|_\infty \\ &\leq \frac{1-\alpha}{AB(\alpha)} \|f(x, y, t)\|_\infty + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \|f(x, y, t)\|_\infty \int_0^t (t-\tau) d\tau \\ &\leq \frac{(1-\alpha)M}{AB(\alpha)} + \frac{\alpha M}{AB(\alpha)\Gamma(\alpha)} \cdot a^\alpha < b. \end{aligned} \quad (6.2.6)$$

This implies that

$$a = \left( \frac{b - \frac{(1-\alpha)M}{AB(\alpha)}}{\frac{\alpha M}{AB(\alpha)\Gamma(\alpha)}} \right)^{\frac{1}{\alpha}}.$$

In what follows, we need to show that the functions  $x(t)$  and  $y(t)$  satisfy a Lipschitz condition. That is

$$\|\Gamma x_1 - \Gamma x_2\|_\infty \leq K \|x_1 - x_2\|_\infty, \quad (6.2.7)$$

which implies

$$\begin{aligned} \Gamma(x_1) &= \frac{1 - \alpha}{AB(\alpha)} f(x_1, y, t) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t f(x_1, y, \tau)(t - \tau)^{\alpha-1} d\tau, \\ \Gamma(x_2) &= \frac{1 - \alpha}{AB(\alpha)} f(x_2, y, t) + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \int_0^t f(x_2, y, \tau)(t - \tau)^{\alpha-1} d\tau, \end{aligned} \tag{6.2.8}$$

so that

$$\begin{aligned} \|\Gamma x_1 - \Gamma x_2\|_\infty &= \frac{1 - \alpha}{AB(\alpha)} \|f(x_1, y, t) - f(x_2, y, t)\|_\infty + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \|f(x_1, y, t) \\ &\quad - f(x_2, y, t)\|_\infty \int_0^t (t - \tau) d\tau \\ &\leq \|f(x_1, y, t) - f(x_2, y, t)\|_\infty \left( \frac{1 - \alpha}{AB(\alpha)} + \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} \cdot \frac{a^\alpha}{\alpha} \right) \\ &\leq \|f(x_1, y, t) - f(x_2, y, t)\|_\infty \left( \frac{1 - \alpha}{AB(\alpha)} + \frac{a^\alpha}{AB(\alpha)\Gamma(\alpha)} \right). \end{aligned} \tag{6.2.9}$$

In other words, if  $f$  is Lipschitz with respect to  $x$ , then

$$\begin{aligned} \|\Gamma x_1 - \Gamma x_2\|_\infty &\leq K \|x_1 - x_2\|_\infty \left\{ \frac{1 - \alpha}{AB(\alpha)} + \frac{a^\alpha}{AB(\alpha)\Gamma(\alpha)} \right\} \\ &\leq L \|x_1 - x_2\|_\infty. \end{aligned} \tag{6.2.10}$$

Similarly,  $g$  is Lipschitz with respect to  $y$  if

$$\|\Gamma y_1 - \Gamma y_2\|_\infty \leq L \|y_1 - y_2\|_\infty. \tag{6.2.11}$$

The procedure given above can be extended to multicomponent system of fractional differential equations.

### 6.3 Numerical Experiments

In this section, we apply the numerical scheme illustrated in the above section to some chaotic systems. The classical time derivative is replaced with the Atangana–Baleanu fractional derivative of order  $\alpha \in (0, 1]$  in the sense of Caputo.

From (6.1.9), we have

$$u_{n+1} = u_n + \omega_1(n, \alpha, h) f(t_n, u_n) + \omega_2(n, \alpha, h) f(t_{n-1}, u_{n-1}), \tag{6.3.1}$$

where

$$\omega_1(n, \alpha, h) = \left\{ \frac{1 - \alpha}{AB(\alpha)} - \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} h^\alpha \left[ \frac{2(n+1)^\alpha}{\alpha} - \frac{(n+1)^{\alpha+1}}{\alpha+1} \right] - \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} h^\alpha \left[ \frac{n^\alpha}{\alpha} - \frac{n^{\alpha+1}}{\alpha+1} \right] \right\}$$

and

$$\omega_2(n, \alpha, h) = f(t_{n-1}, u_{n-1}) \left\{ \frac{\alpha - 1}{AB(\alpha)} - \frac{\alpha}{AB(\alpha)\Gamma(\alpha)} h^\alpha \left[ \frac{(n+1)^\alpha}{\alpha} - \frac{(n+1)^{\alpha+1}}{\alpha+1} + \frac{n^{\alpha+1}}{AB(\alpha)\Gamma(\alpha)h} \right] \right\}.$$

### 6.3.1 Example 1

The following chaotic system is described by the Atangana–Baleanu fractional derivative in the sense of Caputo as

$$\begin{aligned} {}_0^{ABC} \mathcal{D}_t^\alpha x_1(t) &= f_1(x_1, x_2, x_3) = \phi(x_2(t) - x_1(t)) + \sigma x_2(t)x_3(t), \\ {}_0^{ABC} \mathcal{D}_t^\alpha x_2(t) &= f_2(x_1, x_2, x_3) = \varphi x_1(t) - x_1(t)x_3(t), \\ {}_0^{ABC} \mathcal{D}_t^\alpha x_3(t) &= f_3(x_1, x_2, x_3) = x_1(t)x_2(t) - \psi x_3(t) + \delta x_2^2(t), \end{aligned} \tag{6.3.2}$$

where  $x_1(t), x_2(t), x_3(t)$  are the densities or states, and  $\phi, \varphi, \psi, \sigma, \delta$  are positive parameters. From (6.3.1), we have

$$\begin{aligned} x_{1,n+1} &= x_{1,n} + \omega_1(n, \alpha, h) f_1(t_n, x_{1,n}, x_{2,n}, x_{3,n}) \\ &\quad + \omega_2(n, \alpha, h) f_1(t_{n-1}, x_{1,n-1}, x_{2,n-1}, x_{3,n-1}) \\ x_{2,n+1} &= x_{2,n} + \omega_1(n, \alpha, h) f_2(t_n, x_{1,n}, x_{2,n}, x_{3,n}) \\ &\quad + \omega_2(n, \alpha, h) f_2(t_{n-1}, x_{1,n-1}, x_{2,n-1}, x_{3,n-1}) \\ x_{3,n+1} &= x_{3,n} + \omega_1(n, \alpha, h) f_3(t_n, x_{1,n}, x_{2,n}, x_{3,n}) \\ &\quad + \omega_2(n, \alpha, h) f_3(t_{n-1}, x_{1,n-1}, x_{2,n-1}, x_{3,n-1}). \end{aligned}$$

## Reference

1. A. Atangana, K.M. Owolabi, New numerical approach for fractional differential equations. *Math. Modell. Nat. Phenom.* **13**(3), 21 (2018). <https://doi.org/10.1051/mmnp/2018010>

# Chapter 7

## Application to Ordinary Fractional Differential Equations



### 7.1 Numerical Approximation of Fractional Ordinary Differential Equation with the Caputo Derivative

The numerical approximation of classical ordinary differential equations is relatively simple and, being a focus of mathematical studies for the last few decades, has been by now almost completely investigated. However, a fractional case is much less studied and is still poorly understood despite the fact that there has been a growing interest in the research of this area. In short, there has been just handful of research papers and books considering the numerical approximation of time-fractional ordinary differential equations.

Langlands and Henry [15] examined the fractional-order time diffusion equation, and introduced an  $L_1$ -stable scheme for this equation. Sun and Wu [27] derived a finite difference method with  $L_1$  approximation for the fractional-in-time derivative. Lin and Xu [18] construct and analyse a finite difference scheme for the time discretization of the time-fractional diffusion equation, and showed that the time convergence is of order  $2 - \alpha$ . Zhao et al. [30] derived two second-order approximation schemes for time-fractional derivatives involved in anomalous diffusion and wave propagation. Numerical technique for a class of fractional ordinary differential equations was proposed by Kumar and Agrawal [14], in which their approach can be reduced into a Volterra-type integral equation. A general technique for high-order numerical schemes based on this approach is constructed by Cao and Xu [7].

In this chapter, we use the following numerical approximation of the Caputo derivative, which follows closely the work done in [18, 19]. We assume a uniform time step size  $k$ , and let  $t^n = nk$ ,  $n = 0, 1, 2, \dots$ . We also assume  $U^n$  to be the numerical approximation of  $u(t^n)$ .

To derive a first-order method, for  $t = t^{n+1}$ , we assume a uniform partition in time,

$$0 = t_0 < t_1 < t_2 < \dots < t_n < t_{n+1} = t.$$

Next, we approximate each standard time derivative by the forward difference in the form

$$\begin{aligned}
 \partial_t^\alpha u(t^{n+1}) &\approx \frac{1}{\Gamma(1-\alpha)} \sum_{s=0}^n \int_{t_s}^{t_{s+1}} \frac{U^{s+1} - U^s}{k(t_{n+1} - \xi)} d\xi \\
 &= \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \sum_{s=0}^n \frac{(n+1-s)^{1-\alpha} - (n-s)^{1-\alpha}}{k^\alpha} (U^{s+1} - U^s) \\
 &= \frac{1}{\Gamma(2-\alpha)k^\alpha} \left( U^{n+1} - \sum_{n=0}^k d_s^{n+1} U^s \right) \\
 &:= \mathcal{D}_t^\alpha U^{n+1},
 \end{aligned} \tag{7.1.1}$$

where

$$\begin{aligned}
 d_s^{n+1} &= 2(n+1-s)^{1-\alpha} - (n+2-s)^{1-\alpha} - (n-s)^{1-\alpha}, \quad s = 1, 2, \dots, n, \\
 d_0^{n+1} &= (n+1)^{1-\alpha} - n^{1-\alpha}.
 \end{aligned}$$

Bear in mind that  $y = x^{1-\alpha}$  is a concave and increasing function for which  $x > 0$ , by direct calculation, we obtain

$$\sum_{s=0}^n d_s^{n+1} = 1, \quad d_s^{n+1} > 0, \quad s = 0, 1, 2, \dots, n. \tag{7.1.2}$$

Therefore, while the standard time derivative yields the instantaneous rate of change, from its numerical approximation (7.1.1), one can interpret the Caputo derivative as the rate of change of a quantity from a convex combination of its history values, and the coefficients  $d_s^{n+1}$  indicate the influence strength due to the memory effect. As memory effect becomes weaker, the influence strength of a history values decreases in time.

It should be mentioned that, we obtain for a fixed value of order  $\alpha$ ,

$$d_n^{n+1} = 2 - 2^{1-\alpha} - 0^{1-\alpha} = 2 - 2^{1-\alpha},$$

independent of  $n$ . Further, we denote  $d_n^{n+1}$  by  $\hat{d}$  which plays a vital role in the Courant–Friedrichs–Lewy conditions for explicit upwind schemes, as we shall discuss later.

### 7.1.1 Numerical Schemes and Stability Analysis

Here, we adopt the numerical approximation of the Caputo derivative which was introduced in the previous chapter to formulate numerical schemes for ordinary

differential equations, with conservation laws. We focus on examining the stability condition for each scheme and demonstrate how they differ from the models with classical time derivatives.

### 7.1.1.1 Backward Euler Scheme

We consider the time-fractional ODE model

$$\partial_t^\alpha u(t) = \lambda u(t), \quad (7.1.3)$$

where  $\lambda$  is complex number with  $\Re(\lambda) \leq 0$ , which is similar to the eigenvalue of an operator.

The stability analysis of many numerical schemes for ODE in conjunction with the Caputo derivatives has been examined in some previous research materials and books, see, for instance, [5–7, 10, 20]. By applying the backward Euler method for (7.1.3), we have

$$\mathcal{D}_t^\alpha U^{n+1} = \lambda U^{n+1}. \quad (7.1.4)$$

Multiply each side of (7.1.4) by  $k^\alpha \Gamma(2 - \alpha)$ , the above equation becomes

$$(1 - \lambda k^\alpha \Gamma(2 - \alpha)) U^{n+1} = \sum_{s=0}^n d_s^{n+1} U^s.$$

If we let  $z = \lambda k^\alpha \Gamma(2 - \alpha)$ , the stability polynomial  $\pi(\zeta; z)$  for the above scheme is

$$\pi(\zeta; z) = (1 - z)\zeta^{n+1} - \sum_{s=0}^n d_s^{n+1} \zeta^s.$$

In what follows, we discuss various scenarios, that is, when  $\lambda \neq 0$  and when  $\lambda = 0$ .

For the case  $\lambda \neq 0$ , we have  $\Re(z) \leq 0$  and  $z \neq 0$ , then we finally obtain  $|1 - z| > 1$ . If we assume  $\zeta_0$  with  $|\zeta_0| \geq 1$  is a root to  $\pi(\zeta; z)$ , then for  $s \leq n$ , we get

$$|\zeta_0^s| \leq |\zeta_0|^s \leq |\zeta_0^{n+1}|.$$

Then, we obtain

$$\begin{aligned} |(1 - z)\zeta_0^{n+1}| &= |1 - z||\zeta_0|^{n+1} = \left| \sum_{s=0}^n d_s^{n+1} \zeta_0^s \right| \\ &\leq \sum_{s=0}^n d_s^{n+1} |\zeta_0|^s \leq \left( \sum_{s=0}^n d_s^{n+1} \right) |\zeta_0|^{n+1} = |\zeta_0|^{n+1}, \end{aligned}$$

which is a contradiction. This implies that the stability polynomial has only roots with modulus less than 1, and hence the method is absolute stable.

When  $\lambda = 0$ , then  $z = 0$ , and the stability analysis in this case reduces to the zero stability of the time discretization. If the modulus of the root of the stability polynomial is unity, that is, 1, we assume that the root is  $\zeta_0 = e^{i\theta}$ .

If  $\zeta = 0$ , then  $\eta_0 = 1$ , so that

$$\pi(1; 0) = 1^{n+1} - \sum_{s=0}^n d_s^{n+1} = 0,$$

and we compute

$$\frac{d\pi(\zeta; 0)}{d\zeta} = (n+1)\zeta^n - \sum_{s=0}^n d_s^{n+1} s \zeta^{s-1}.$$

The coefficients  $\{d_s^{n+1}\}_{s=0}^n$  satisfy (7.1.2), and therefore

$$\left| \sum_{s=0}^n d_s^{n+1} s \right| < \left| \sum_{s=0}^n d_s^{n+1} n \right| = n.$$

We can now conclude that

$$\frac{d\pi}{d\zeta} = (n+1) - \sum_{s=0}^n d_s s > n+1 = 1 \neq 0.$$

Hence, 1 is not a repeated root of the stability polynomial.

If  $\theta \neq 0$ , then we obtain the following equation:

$$e^{i(n+1)\theta} = \sum_{s=0}^n d_s^{n+1} e^{is\theta}.$$

We divide each side by  $e^{i(n+1)\theta}$  to have

$$\sum_{s=0}^n d_s^{n+1} e^{i(s-1-n)\theta}.$$

Since  $\theta \neq 0$ , at least one  $e^{i(s-1-n)\theta}$  is not real valued. Then, the right-hand side of the above equation is a convex combination of  $n+1$  unit complex numbers. Hence,  $e^{i\theta}$  with  $\theta \neq 0$  is not a root to the stability polynomial.

### 7.1.1.2 Explicit Upwind Scheme for the Scalar Conservation Law

#### The First-Order Method

We consider the one-dimensional conservation law

$$\partial_t^\alpha u + (g(u))_x = 0, \quad (7.1.5)$$

where the flux function is decomposed as

$$g = g^+ + g^-, \quad (g^+)' \geq 0, \quad (g^-)' \leq 0.$$

The above assumption is made to simplify our analysis. It should be noted that the flux decomposition is not the major requirement for designing such numerical methods. For general discussion on this issue, we refer our readers to [19, 29]. Without loss of generality, the flux function  $g(u)$  could either be linear or nonlinear. But obviously, it also involves the linear advection case, when  $g = \sigma u$ .

Likewise, we assume a uniform time step  $k$ , and let  $t^n = nk$ ,  $n = 0, 1, 2, \dots$ . In addition, on the computational interval  $[a, b]$ , we assume uniform spatial grids  $x_j = \sigma + jh$ , for  $j = 0, 1, 2, \dots, N$ , with spatial grid size  $h = \frac{b-a}{N}$ . Let  $U_j^k$  be the numerical approximation of  $u(x = x_j, t = t^s)$ , then the first-order upwind scheme for the nonlinear conservation law is given as

$$\mathcal{D}_t^\alpha U_j^{n+1} + \frac{1}{h} \{g^+(U_j^n) - g^+(U_{j-1}^n)\} + \frac{1}{h} \{g^-(U_{j+1}^n) - g^-(U_j^n)\} = 0. \quad (7.1.6)$$

If we let

$$\lambda_j^{+,n} = \frac{\sigma_j^{+,n} k^\alpha \Gamma(2-\alpha)}{h} \quad \text{and} \quad \lambda_j^{-,n} = \frac{\sigma_j^{-,n} k^\alpha \Gamma(2-\alpha)}{h},$$

where for some  $\zeta_j^n$  between  $U_{j-1}^n$  and  $U_j^n$  and some  $\mu_j^n$  between  $U_j^n$  and  $U_{j+1}^n$ , we obtain

$$\begin{aligned} \sigma_j^{+,n} &= \frac{g^+(u_j^n) - g^+(u_{j-1}^n)}{U_j^n - U_{j-1}^n} = (f^+)'(\zeta_j^n) \geq 0, \\ \sigma_j^{-,n} &= \frac{g^-(u_{j+1}^n) - g^-(u_j^n)}{U_{j+1}^n - U_j^n} = (f^-)'(\mu_j^n) \leq 0, \end{aligned}$$

then, we rewrite the numerical scheme as

$$U_j^{n+1} = \left(\bar{d} - \lambda_j^{+,n} + \lambda_j^{-,n}\right) U_j^n + \lambda_j^{+,n} U_{j-1}^n - \lambda_j^{-,n} U_{j+1}^n + \sum_{s=0}^{n-1} d_s^{n+1} U_j^s, \quad (7.1.7)$$

we therefore propose the CFL condition for the first-order upwind scheme as

$$\frac{k^\alpha \Gamma(2 - \alpha)}{h} \left\{ \max |(g^+)'| + \max |(g^-)'| \right\} \leq \bar{d}. \quad (7.1.8)$$

The CFL condition is observed to be essentially agreed with the conservation law and standard time derivatives, exception is that the time step  $k$  gains an exponent  $\alpha$  due to the Caputo derivative.

With the CLF condition, we obtain

$$\bar{d} - \lambda_j^{+,n} + \lambda_j^{-,n} \geq 0.$$

Therefore, we say that the maximum principle for the upwind scheme,  $\forall n \in \mathbb{N}^+$

$$\max_j |U_j^n| \leq \lim_j |U_j^0|.$$

In addition, we can verify that this scheme is total variation diminishing (TVD) if the CFL condition (7.1.8) holds. In actual sense, we can rewrite (7.1.7) in the form

$$U_j^{n+1} = \bar{d}U_j^n - \rho g^+(U_j^n) + \rho g^+(U_j^n) + \rho g^+(U_{j-1}^n) - \rho g^+(U_{j+1}^n) + \sum_{s=0}^{n-1} d_s^{n+1} U_j^s, \quad (7.1.9)$$

where  $\rho = \frac{k^\alpha \Gamma(2-\alpha)}{h}$ . Next, we consider another solution, say  $Z$ , satisfying the same difference equation

$$Z_j^{n+1} = \bar{d}Z_j^n - \rho g^+(Z_j^n) + \rho g^+(Z_j^n) + \rho g^+(Z_{j-1}^n) - \rho g^+(Z_{j+1}^n) + \sum_{s=0}^{n-1} d_s^{n+1} Z_j^s. \quad (7.1.10)$$

On subtracting (7.1.10) from (7.1.9), we have

$$\begin{aligned} U_j^{n+1} - Z_j^{n+1} &= \bar{d}(U_j^n - Z_j^n) - \rho(g^+(U_j^n) - g^+(Z_j^n)) + \rho(g^-(U_j^n) - g^-(Z_j^n)) \\ &\quad + \rho(g^+(U_{j-1}^n) - g^+(Z_{j-1}^n)) - \rho(g^-(U_{j+1}^n) - g^-(Z_{j+1}^n)) \\ &\quad + \sum_{s=0}^{n-1} d_s^{n+1} (U_j^s - Z_j^s). \end{aligned}$$

Then, by adopting the mean value theorem, we get

$$\begin{aligned} U_j^{n+1} - Z_j^{n+1} &= \left[ \bar{d} - \rho(g^+)'(\zeta_j^+) + \rho(g^-)'(\zeta_j^-) \right] (U_j^n - Z_j^n) + \rho(g^+)'(\zeta_{j-1}^+) (U_{j-1}^n - Z_{j-1}^n) \\ &\quad - \rho(g^-)'(\zeta_{j+1}^-) (U_{j+1}^n - Z_{j+1}^n) + \sum_{s=0}^{n-1} d_s^{n+1} (U_j^s - Z_j^s), \end{aligned}$$

where  $\zeta_j^+$  and  $\zeta_j^-$  are the numbers between  $U_j^n$  and  $Z_j^n$ , respectively. When the CFL condition in (7.1.8) is held, we get

$$\bar{d} - \rho(g^+) (\zeta_j^+) + \rho(g^-) (\zeta_j^-) \geq 0.$$

By triangle inequality, we have

$$\begin{aligned} &|U_j^{n+1} - Z_j^{n+1}| \\ &= \left[ \bar{d} - \rho(g^+) (\zeta_j^+) + \rho(g^-) (\zeta_j^-) \right] (U_j^n - Z_j^n) + \rho(g^+) (\zeta_{j-1}^+) |U_{j-1}^n - Z_{j-1}^n| \\ &\quad - \rho(g^-) (\zeta_{j+1}^-) |U_{j+1}^n - Z_{j+1}^n| + \sum_{s=0}^{n-1} d_s^{n+1} |U_j^k - Z_j^k|. \end{aligned}$$

Summing the equation over  $j$  gives

$$\sum_j |U_j^{n+1} - Z_j^{n+1}| \leq \sum_{s=0}^n d_s^{n+1} \sum |U_j^s - Z_j^s|.$$

One observed here that the flux terms have been removed. By induction, we have

$$\|U^n - Z^n\|_{\ell^1} \leq \|U^0 - Z^0\|_{\ell^1},$$

as the desired result for the following theorem.

**Theorem 7.1.1** *The first-order upwind scheme (7.1.6) for the scalar conservative law,*

$$\partial_t^\alpha u(x, t) + g(u(x, t))_x = 0, \quad x \in \mathbb{R}, \quad t > 0,$$

*is  $\ell^1$  contracting, when the CFL condition (7.1.8) holds.*

## 7.2 Modelling the Spread of Viruses in Computer via the Caputo Fractional Derivative

In this example, we consider a modified form of an epidemiological model for the spread of viruses in computer as proposed by Piqueira and Araujo [24]. In their report, the total population of this model is represented by  $T$  which is broken down into four different groups.  $S$  stands for the non-infected computers capable of being infected after making contact with infected computer.  $A$  denotes the type of non-infected computer systems that are equipped with antivirus. Infected computers that

are capable of infecting non-infected computers are given by  $I$  and  $R$  accounts for the removed ones due to infection or non-infection. The recruitment rate of computers into the non-infected systems' class is represented by  $N$  and  $\mu$  is the proportion coefficient for the death rate which is not attributed to the virus. The rate of infection due to product  $SI$  is given by  $\beta$ . The conversion of susceptible system into antidotal is the product of  $SI$  given by  $\alpha_{AS}$ . The proportion of converting infected computer systems into antidotal ones in the network is the product of  $AS$  denoted by  $\alpha_{AI}$ . The rate of removed computers being converted into susceptible class is denoted by  $\sigma$ , and  $\delta$  connotes the rate at which the virus renders the computers useless and remove from the system.

The mathematical model describing the spread of viruses in computer systems is given as

$$\begin{aligned}\frac{dS}{dt} &= N - \alpha_{AS}SA - \beta SI - \mu S + \sigma R, \\ \frac{dI}{dt} &= \beta SI - \alpha_{AI}AI - \delta I - \mu I \\ \frac{dR}{dt} &= \delta I - \sigma R - \mu R, \\ \frac{dA}{dt} &= \alpha_{AS}SA + \alpha_{AS}AI - \mu A.\end{aligned}\tag{7.2.1}$$

For this example, the recruitment rate is let to be  $N = 0$ , which means that there is no new computer entering into the system during the spread of the virus. This is because in real life the spread of virus in computer machines is much more faster than adding new computers into the system. The same reason goes for the choice of taking  $\mu = 0$ , bearing in mind the fact that the computer system outmodedness time is longer than the time of the virus action being manifested.

In accordance with the above information, we reformulate equation (7.2.1) to become

$$\begin{aligned}\frac{dS}{dt} &= -\alpha_{AS}SA - \beta SI + \sigma R, \\ \frac{dI}{dt} &= \beta SI - \alpha_{AI}AI - \delta I \\ \frac{dR}{dt} &= \delta I - \sigma R, \\ \frac{dA}{dt} &= \alpha_{AS}SA + \alpha_{AS}AI.\end{aligned}\tag{7.2.2}$$

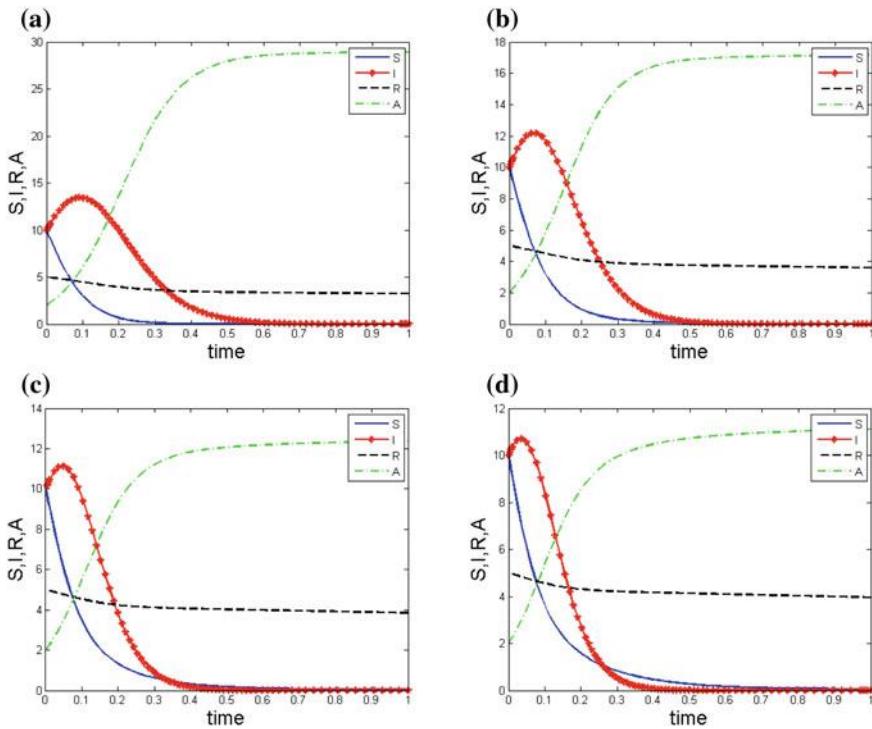
In the context of fractional derivative, Eq.(7.2.2) can be written in the form

$$\begin{aligned}
 {}_0^C \mathcal{D}_t^\alpha S(t) &= -\alpha_{AS}SA - \beta SI + \sigma R, \\
 {}_0^C \mathcal{D}_t^\alpha I(t) &= \beta SI - \alpha_{AI}AI - \delta I \\
 {}_0^C \mathcal{D}_t^\alpha R(t) &= \delta I - \sigma R, \\
 {}_0^C \mathcal{D}_t^\alpha A(t) &= \alpha_{AS}SA + \alpha_{AS}AI,
 \end{aligned}
 \tag{7.2.3}$$

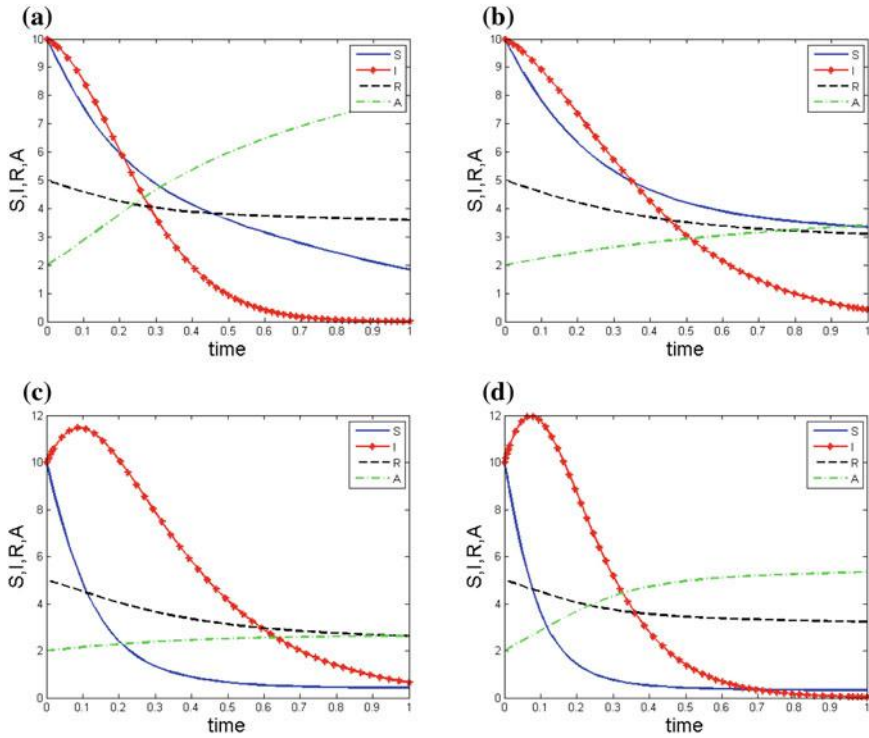
where  ${}_0^C \mathcal{D}_t^\alpha$  remains the Caputo derivative as discussed in the previous chapter.

The fractional derivative is known for non-local problems and can be appropriate for modelling epidemiological issues. The fractional order in the above system, however, is an important tool for numerical experiments. Hence, to model the spread of the computer virus in a network, a local derivative with fractional order is considered. Before going to the numerical simulations, we briefly present the linear stability analysis of the model. In order to give guidelines on the correct choice of parameters for numerical simulation of the full fractional system, it is important to consider the system at

$${}_0^C \mathcal{D}_t^\alpha S(t) = {}_0^C \mathcal{D}_t^\alpha I(t) = {}_0^C \mathcal{D}_t^\alpha R(t) = {}_0^C \mathcal{D}_t^\alpha A(t) = 0.$$



**Fig. 7.1** Approximate solution for system (7.2.3) at  $\alpha = 0.89$  and some instances of  $\alpha_{IA}$  which correspond to **a**  $\alpha_{IA} = 0.4$ , **b**  $\alpha_{IA} = 0.8$ , **c**  $\alpha_{IA} = 1.4$  and **d**  $\alpha_{IA} = 1.8$  with simulation time  $t = 1.0$ . Take note of the variation in amplitudes



**Fig. 7.2** Approximate solution for system (7.2.3) at  $\alpha = 0.93$  and some instances of  $\alpha_{AS}$  and simulation time  $t = 1.0$ . Other parameters are  $\alpha_{AI} = 1.4$ ,  $\beta = 0.25$ ,  $\sigma = 0.085$  and  $\delta = 0.4$ . Panels (a-d) correspond to  $\alpha_{AS} = 0.2$ ,  $\alpha_{AS} = 0.25$ ,  $\alpha_{AS} = 0.04$  and  $\alpha_{AS} = 0.06$ , respectively

So that

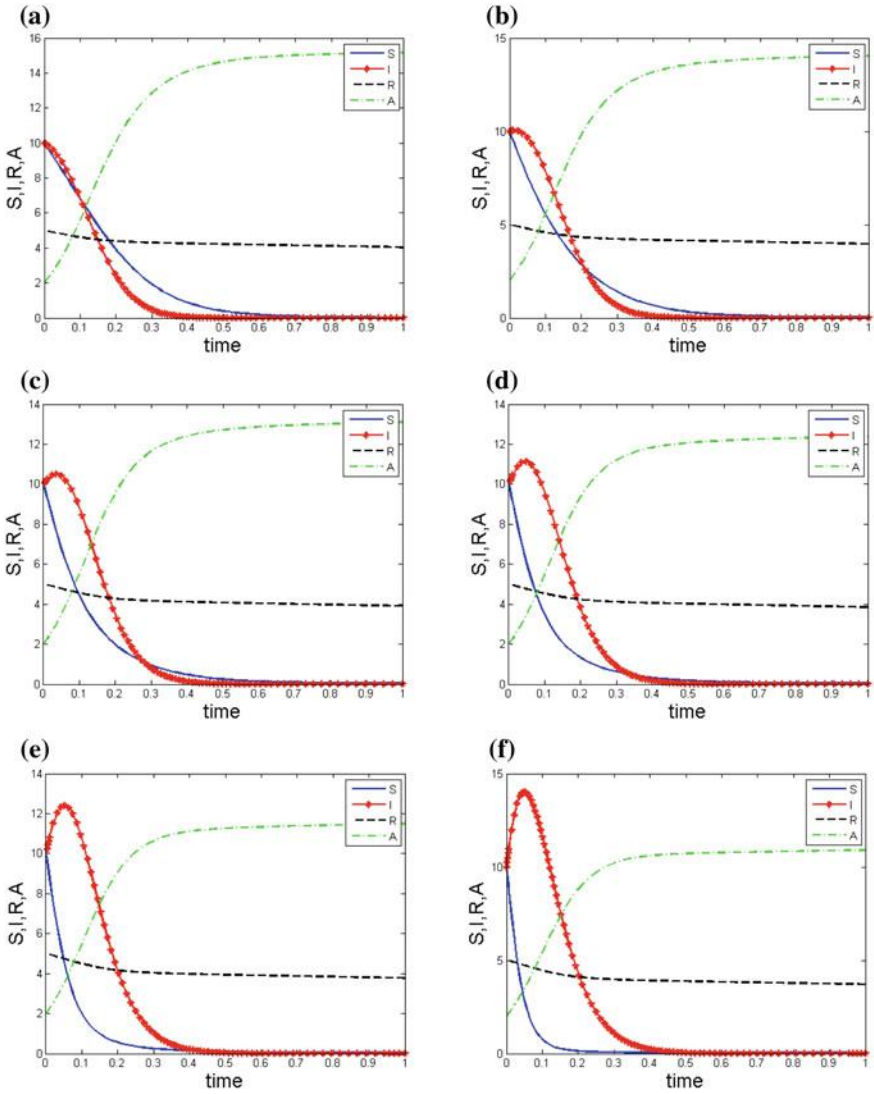
$$\begin{aligned}
 0 &= -\alpha_{AS}S^*A^* - \beta S^*I^* + \sigma R^*, \\
 0 &= \beta S^*I^* - \alpha_{AI}A^*I^* - \delta I^* \\
 0 &= \delta I^* - \sigma R^*, \\
 0 &= \alpha_{AS}S^*A^* + \alpha_{AS}A^*I^*.
 \end{aligned} \tag{7.2.4}$$

On solving, the above equation gives

$$S^* = \frac{\delta}{\beta}, \quad I^* = \frac{T - \delta/\beta}{1 + \delta/\sigma}, \quad R^* = \frac{T - \delta/\beta}{1 + \sigma/\delta}, \quad A^* = 0. \tag{7.2.5}$$

The disease-free equilibria are calculated as

$$E_a = (S, I, R, A) = (0, 0, 0, T)$$



**Fig. 7.3** Approximate solution for system (7.2.3) showing the effect of  $\beta$  at  $\alpha = 0.90$ . Plots **a–f**  $\beta = 0.2, \beta = 0.4, \beta = 0.6, \beta = 0.8, \beta = 1.2$  and  $\beta = 1.85$ , respectively, with simulation time  $t = 1.0$ . Other parameters are given in Fig. 7.2

and

$$E_b = (S, I, R, A) = (T, 0, 0, 0).$$

For details on stability analysis of this model, readers are referred to [24].

For the numerical experiments, computation is done with parameters in [24] to obtain different results for values of fractional power  $\alpha$  and time  $t$ . The parameters applied here are  $\alpha_{AS} = 0.6, \alpha_{IA} = 0.4, \beta = 0.2, \sigma = 0.85$  and  $\delta = 0.4$ , with the initial conditions  $S(0) = 10, I(0) = 10, R(0) = 5$  and  $A(0) = 20$ .

Figure 7.1 shows the graphical illustration of system (7.2.3) at  $\alpha = 0.89$  and some instances of  $\alpha_{IA}$  which denotes the proportional rate of converting infected computers into antidotal ones in the network due to product of  $SA$ . It is obvious from the graph that the susceptible group which represents the total population quickly gets infected due to the rate at which the virus spreads in the system. So, the figures clearly show that the total number of infected computer machines decreased as the total number of antidotal increased which is a technique to minimize the number of susceptible computer systems. Obviously, the number of non-infected computers is increasing in the amplitudes regardless of the rate  $\alpha_{AI}$ .

In Fig. 7.2, by varying  $\alpha_{AS}$ , which represents the conversion of susceptible system into antidotal due to the product of  $SI$ , we observed decrease in the classes  $S, I, R$  at  $\alpha = 0.93$ . The numerical prediction obtained in Fig. 7.3 is attributed to fractional order  $\alpha = 0.90$  at  $t = 1.0$ . In reality, we observed that by increasing the number of computers that are well equipped with antivirus would definitely reduce the spread of such virus, as depicted in Fig. 7.3a–f. Thus, this application has given a better prediction of how a virus spread can be checked among the computer users.

### 7.3 Modelling the Spread of River Blindness Disease with the Caputo Fractional Derivative

For the second experiment, consideration is given to the mathematical model

$$\begin{aligned} \frac{dA_S(t)}{dt} &= \psi + \delta_A B_I + \alpha\beta A_I - \xi A_S B_I - \tau_A A_S \\ \frac{dA_I(t)}{dt} &= A_S B_I - \delta_I H_I - \alpha\beta A_I - \xi A_S B_I - \tau_I H_I, \\ \frac{dB_I(t)}{dt} &= \delta_B A_I - \rho_I B_I - \gamma B_S, \\ \frac{dB_S(t)}{dt} &= \delta B_S - \rho_I B_I - \delta_A B_I, \end{aligned} \tag{7.3.1}$$

which is used to describe the spread of river blindness disease [2].

Some of the areas that are naturally endowed with rivers are found in the tropical zones covered by the Central and West African nations. Most of these areas are seriously ravaged by poverty which lead most dwellers to depend solely on the use of water from the rivers. A typical example can be drawn from most villages in Chad and Cameroon where people use river water for bathing, drinking and other domestic purposes. It should be noted that water from these rivers is not always healthy and safe which may often result in diseases. One of the most common diseases found in these areas is known as the onchocerciasis. Onchocerciasis is referred to as river blindness and Robbes disease, which is an infectious disease arising from infection with the parasitic worm *Onchocerca volvulus* [28]. This disease is the second-most cause of blindness due to infection, after trachoma [28]. The causative agent of this parasite is the spread by the bites of black flies of the genus *Simulium* that lives near rivers. Once the host is affected, the worm produces larvae that make their way back out to the skin, where they can infect the next black fly that can bite another person. A report presented in [22] has shown that multiple bites are required for infection to occur.

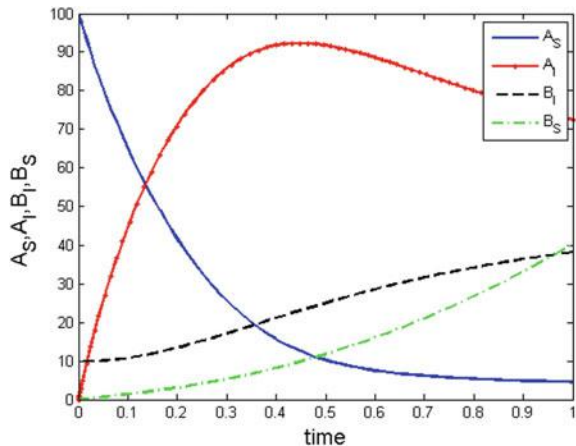
Owing to the privilege granted by the concept of fractional derivative, we extend model (7.3.1) within the scope of the Caputo fractional derivative. Hence, the fractional form of the above model becomes

$$\begin{aligned}
 {}_0^C \mathcal{D}_t^\alpha A_S(t) &= \psi + \delta_A B_I + \alpha \beta A_I - \xi A_S B_I - \tau_A A_S \\
 {}_0^C \mathcal{D}_t^\alpha A_I(t) &= A_S B_I - \delta_I H_I - \alpha \beta A_I - \xi A_S B_I - \tau_I H_I, \\
 {}_0^C \mathcal{D}_t^\alpha B_I(t) &= \delta_B A_I - \rho_I B_I - \gamma B_S, \\
 {}_0^C \mathcal{D}_t^\alpha B_S(t) &= \delta B_S - \rho_I B_I - \delta_A B_I,
 \end{aligned}
 \tag{7.3.2}$$

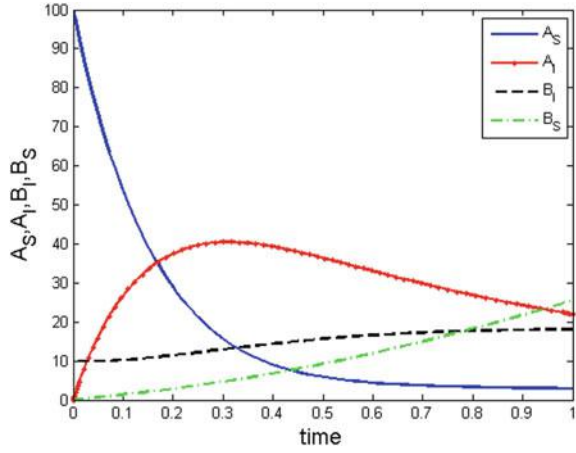
where  ${}_0^C \mathcal{D}_t^\alpha$  is the Caputo fractional derivative of order  $\alpha \in [0, 1]$

The theoretical parameters used for the simulation are given in the following table. Effects of fractional power  $\alpha$  are verified in Figs. 7.4, 7.5 and 7.6. In the experiment,

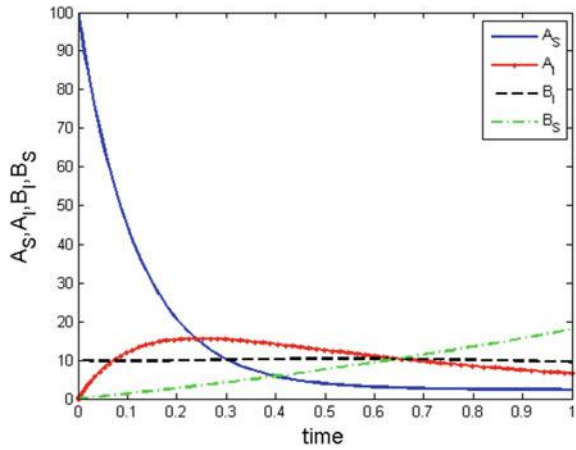
**Fig. 7.4** Approximate solution for fractional system (7.3.2) at  $\alpha = 0.45$  and simulation time  $t = 1.0$



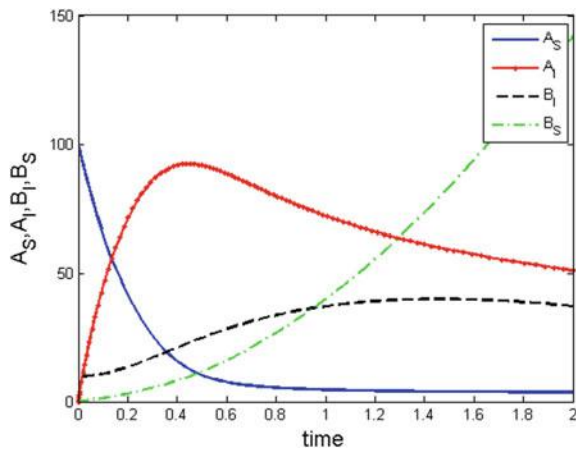
**Fig. 7.5** Approximate solution for fractional system (7.3.2) at  $\alpha = 0.75$  and simulation time  $t = 1.0$



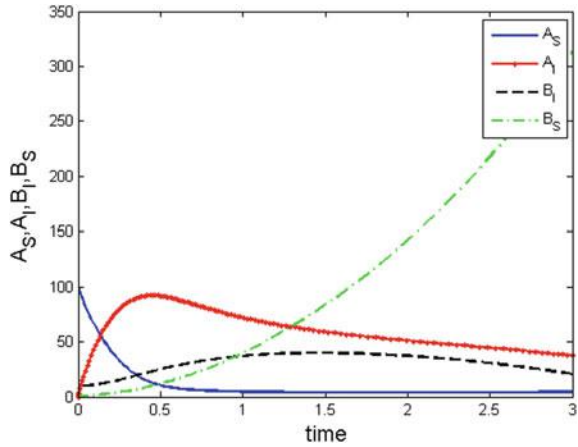
**Fig. 7.6** Approximate solution for fractional system (7.3.2) at  $\alpha = 0.91$  and simulation time  $t = 1.0$



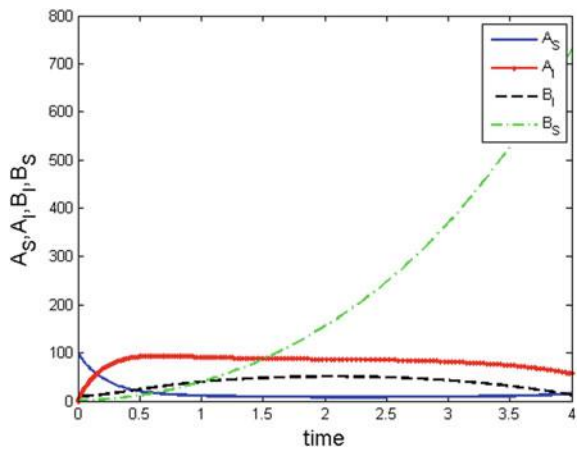
**Fig. 7.7** Approximate solution for fractional system (7.3.2) at  $\alpha = 0.53$  and simulation time  $t = 2.0$



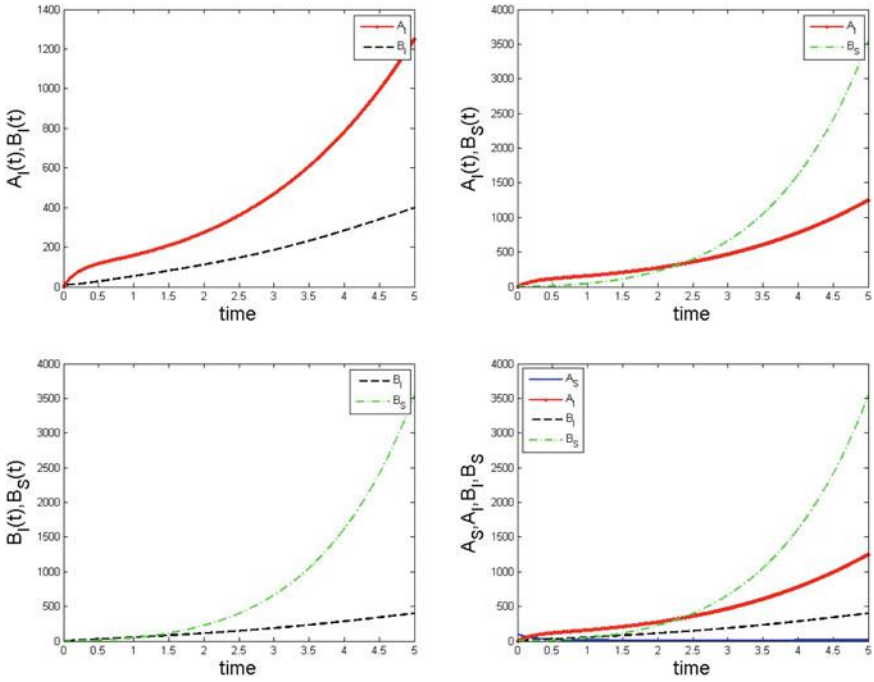
**Fig. 7.8** Approximate solution for fractional system (7.3.2) at  $\alpha = 0.53$  and simulation time  $t = 3.0$



**Fig. 7.9** Approximate solution for fractional system (7.3.2) at  $\alpha = 0.53$  and simulation time  $t = 4.0$



we observed that an increase in the value of  $\alpha$  corresponds to a decrease in the amplitude of class  $A_I$ . In Figs. 7.7, 7.8 and 7.9, we fixed  $\alpha = 0.53$  and varied  $t$  to examine the effect of time. It was observed that increase in time results in the increase of the amplitude of class  $B_S$ . Numerical simulation of fractional system (7.2.3) at  $\delta_I = 0.09$  and  $\alpha = 0.38$  for a bigger time  $t = 5.0$  is given in Fig. 7.10. Clearly, classes  $A_I, B_I, B_S$  give rise to amplitudes.



**Fig. 7.10** Numerical solution for system (7.2.3) at  $\alpha = 0.38$ ,  $\delta_I = 0.09$  and time  $t = 5$ . Other parameters are given in Table 7.1

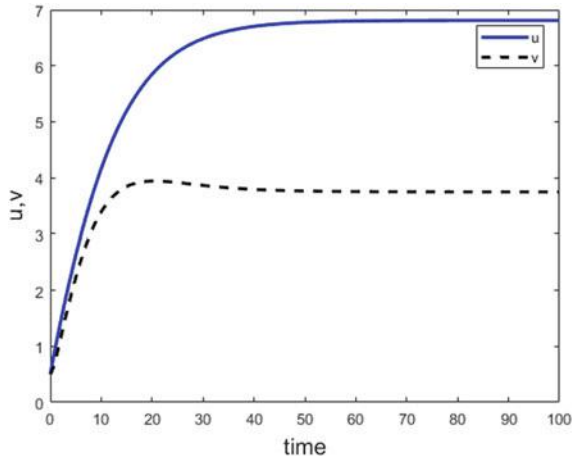
**Table 7.1** Theoretical parameters

Parameters	Values	Parameters	Values
$A_S(0)$	100	$\delta_A$	0.6
$A_I(0)$	0	$\delta_I$	0.9
$B_S(0)$	10	$\delta_B$	0.6
$B_I(0)$	0	$\tau_A$	0.6
$\gamma$	1	$\tau_I$	0.5
$\beta$	0.5	$\rho_I$	0.7
$\delta$	1	$\psi$	10
$\xi$	0.4		

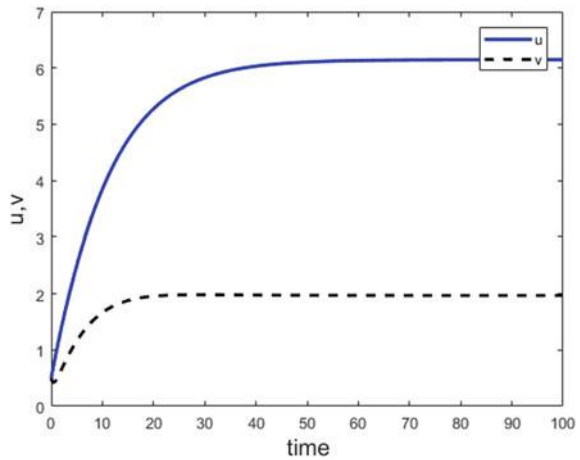
### 7.4 Modelling of Nonlinear Interpersonal Relationship with Time-Fractional Derivative

Mathematical models have been used to describe many physical real-life problems encountered in natural sciences, such as biology, chemistry, physics and astronomy, to mention a few. Research has also been conducted on interpersonal relationships

**Fig. 7.11** Approximate solution for time-fractional system (7.4.1) at  $\alpha = 0.25$



**Fig. 7.12** Approximate solution for time-fractional system (7.4.1) at  $\alpha = 0.35$



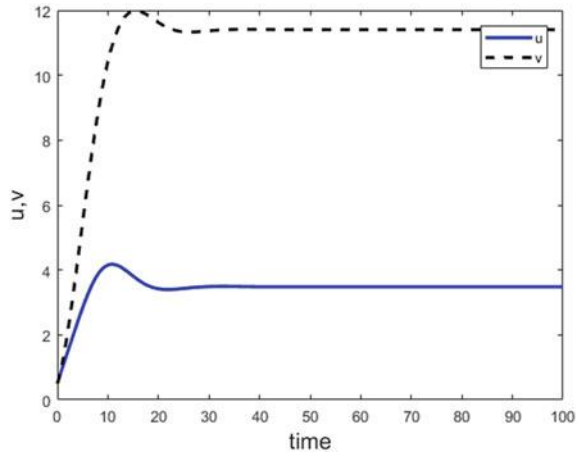
by some authors, for instance, Strogatz [26], Ozalp and Koca [23] with many other references given by Koca and Atangana [12].

The time-fractional version of interpersonal relationship model is given as

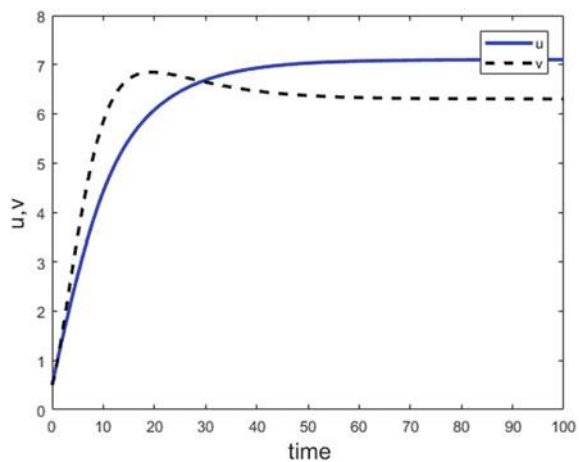
$$\begin{aligned}
 {}_0^A \mathcal{D}_t^\alpha u(t) &= -\phi_1 u + \varphi_1 v(1 - \xi v^2) + \omega_1, \\
 {}_0^A \mathcal{D}_t^\alpha v(t) &= -\phi_2 v + \varphi_2 u(1 - \xi u^2) + \omega_2,
 \end{aligned}
 \tag{7.4.1}$$

subject to initial conditions  $u(0) = 0$  and  $v(0) = 0$ , for  $x \geq a$ ,  $\alpha \in [0, 1]$ . The above alpha derivative is given as

**Fig. 7.13** Approximate solution for time-fractional system (7.4.1) at  $\alpha = 0.55$



**Fig. 7.14** Approximate solution for time-fractional system (7.4.1) at  $\alpha = 0.48$

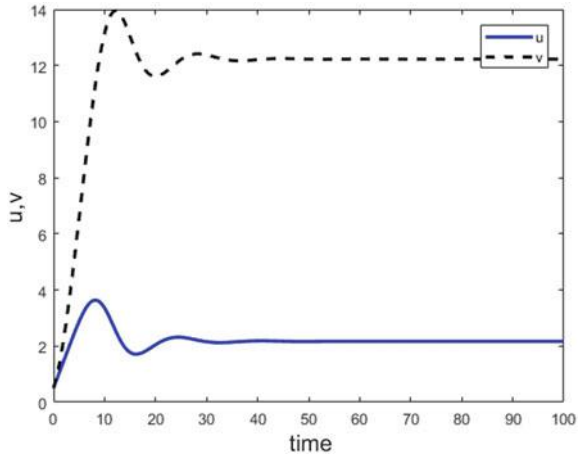


$${}^A_0\mathcal{D}_t^\alpha(f(x)) = \lim_{\delta \rightarrow 0} \frac{f\left(x + \delta\left(x + \frac{1}{\Gamma(\alpha)}\right)^{1-\alpha}\right) - f(x)}{\delta},$$

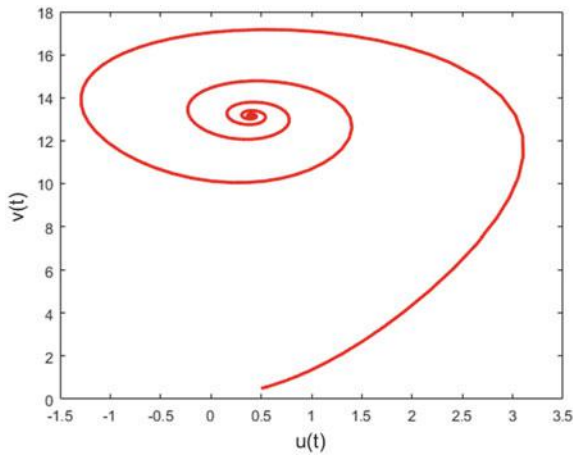
for  $x \geq a, \alpha \in [0, 1]$ . Then if the limit exists,  $f$  is  $\alpha$ -differentiable.

In the above model  $\phi_i > 0, \phi_i, \varphi_i$  and  $\omega_i$  for  $i = 1, 2$  are real constants. These parameters are considered to be oblivion, reaction and attraction constants. In the system above, we assume that feelings decay or degenerate faster in exponential manner in the absence of partners. The variables  $u, v$  represent the measure of romantic style of the individuals. For example,  $\phi_i$  denote the rate at which individual  $i$  is encouraged by his or her own feeling. That is to say,  $i$  represents the degree to which an individual has internalized a sense of his or her self-worth. The parameters  $\varphi_i$  denotes the rate at which individual  $i$  is encouraged by his or her partner, and/or expects his/her

**Fig. 7.15** Approximate solution for time-fractional system (7.4.1) at  $\alpha = 0.87$



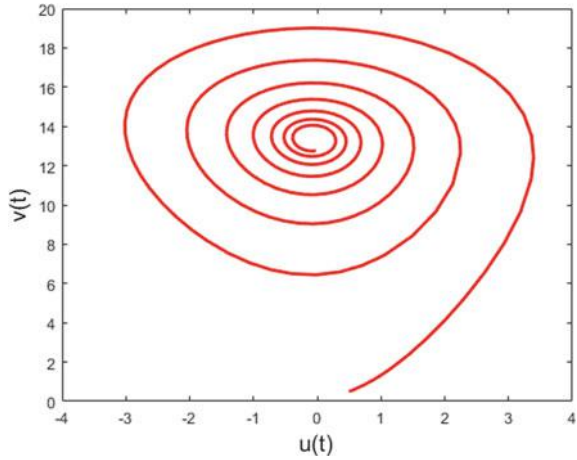
**Fig. 7.16** Individuals attraction for time-fractional system (7.4.1) when  $\alpha = 0.68$



partner to be supportive. In a nutshell, the terms  $-\phi_i u$  and  $-\phi_i v$  suggest that the love measure of  $u$  and  $v$  in the absence of the partner decay exponentially and  $\frac{1}{\phi_i}$  is the required time for love to decay.

For the numerical simulations as shown in Figs. 7.11, 7.12, 7.13, 7.14, 7.15, 7.16 and 7.17, we use the initials  $u(0) = 0.5$ ,  $v(0) = 0.5$  and the parameter values  $\phi_1 = 0.1$ ,  $\phi_2 = 0.04$ ,  $\varphi_1 = 0.005$ ,  $\varphi_2 = 0.001$ ,  $\xi = 0.01$ ,  $\omega_1 = 0.02$  and  $\omega_2 = 0.03$  with simulation time  $t = 100$ . Results for different values of  $\alpha$  showing the relationship between individuals  $u$  and  $v$  are presented in Figs. 7.11, 7.12, 7.13, 7.14 and 7.15. The attraction between these individuals at two instances of fractional power is depicted in Figs. 7.16 and 7.17.

**Fig. 7.17** Individuals attraction for time-fractional system (7.4.1) when  $\alpha = 0.83$



### 7.5 Modelling of El Niño Chaotic Dynamical System with the Caputo, Caputo–Fabrizio and Atangana–Baleanu Fractional Derivatives

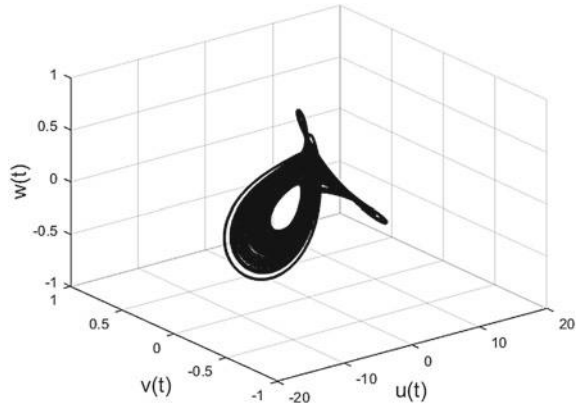
The classical El Niño chaotic dynamical system is given by

$$\begin{aligned} \frac{du(t)}{dt} &= \beta v(t) - \gamma u(t) + \gamma \rho, \\ \frac{dv(t)}{dt} &= u(t)w(t) - v(t), \\ \frac{dw(t)}{dt} &= -u(t)v(t) - w(t) + 1, \end{aligned} \tag{7.5.1}$$

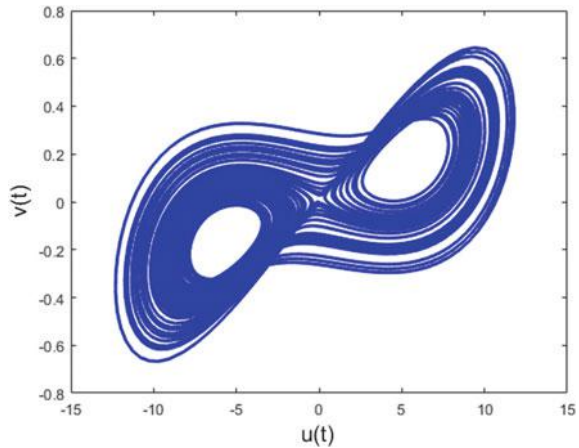
which has been used to describe a very useful physical problem. Chaotic system (7.5.1) has been used to describe an anomalous, devilish irregular and Christmas-time warming of the Peru and Ecuador coastal waters that occurs roughly about every 3–6 years, which has a great impact on global climate. Though the model has been applied with significant degrees of success, irregular and anomalous phenomena cannot be adequately described with the local or classical derivatives, which has been suggested in many research papers, books and monographs [8, 9, 25]. Hence, for a more accurate representation, we present the Caputo and Caputo–Fabrizio forms of (7.5.1) as

$$\begin{aligned} {}_0^C \mathcal{D}_t^\alpha u(t) &= \beta v(t) - \gamma u(t) + \gamma \rho, \\ {}_0^C \mathcal{D}_t^\alpha v(t) &= u(t)w(t) - v(t), \\ {}_0^C \mathcal{D}_t^\alpha w(t) &= -u(t)v(t) - w(t) + 1, \end{aligned} \tag{7.5.2}$$

**Fig. 7.18** Three-dimensional representation of chaotic system (7.5.2) for  $\alpha = 0.92$  and  $t = 100$



**Fig. 7.19** Two-dimensional plot of  $u(t)$  and  $v(t)$  of chaotic system (7.5.2) for  $\alpha = 0.92$  and  $t = 100$

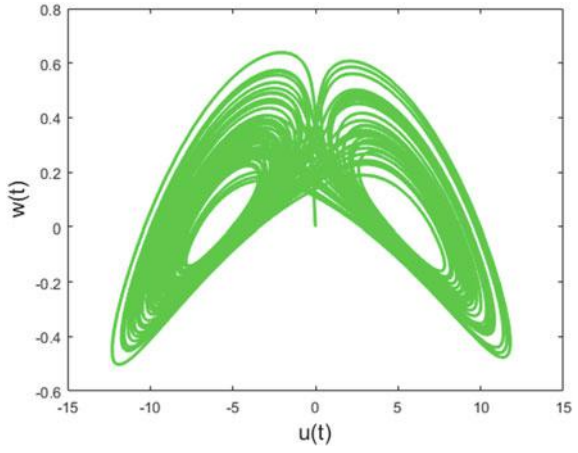


and

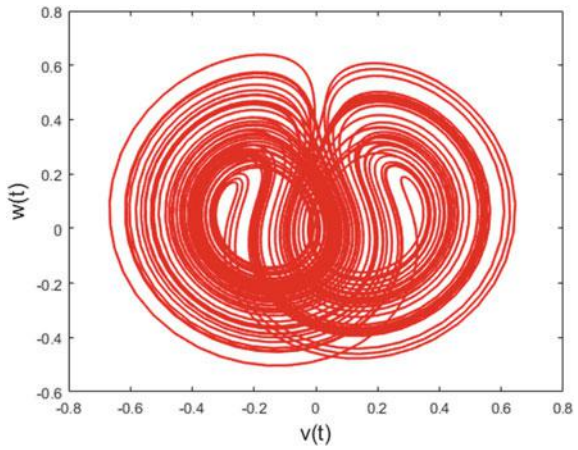
$$\begin{aligned}
 {}_0^CF \mathcal{D}_t^\alpha u(t) &= \beta v(t) - \gamma u(t) + \gamma \rho, \\
 {}_0^CF \mathcal{D}_t^\alpha v(t) &= u(t)w(t) - v(t), \\
 {}_0^CF \mathcal{D}_t^\alpha w(t) &= -u(t)v(t) - w(t) + \kappa,
 \end{aligned}
 \tag{7.5.3}$$

respectively, where  $\beta, \gamma, \rho$  and  $\kappa$  are positive parameters. Here, we simulate the El Niño chaotic dynamical system using both the Caputo derivative with power-law kernel which has singularity and the Caputo–Fabrizio derivative with the exponential law which has no singularity. A non-local and non-singular kernel version was combined by the Atangana–Baleanu fractional derivative. The initial and parameters are given as  $u(0) = v(0) = w(0) = 0, \beta = 102, \gamma = 3, \rho = 0.45$  and  $\kappa = 1$ .

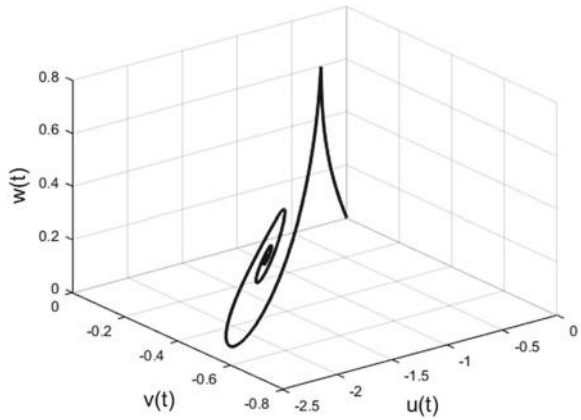
**Fig. 7.20** Two-dimensional plot of  $u(t)$  and  $w(t)$  of chaotic system (7.5.2) for  $\alpha = 0.92$  and  $t = 100$



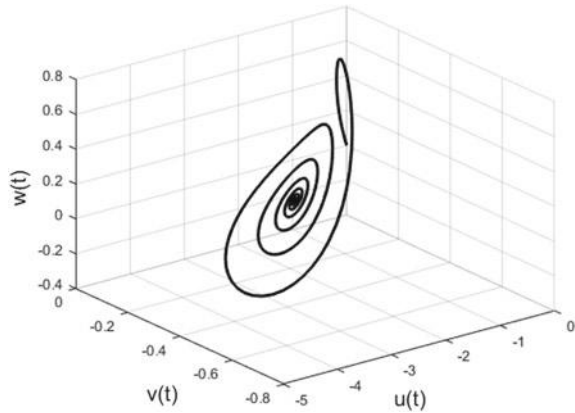
**Fig. 7.21** Two-dimensional plot of  $v(t)$  and  $w(t)$  of chaotic system (7.5.2) for  $\alpha = 0.92$  and  $t = 100$



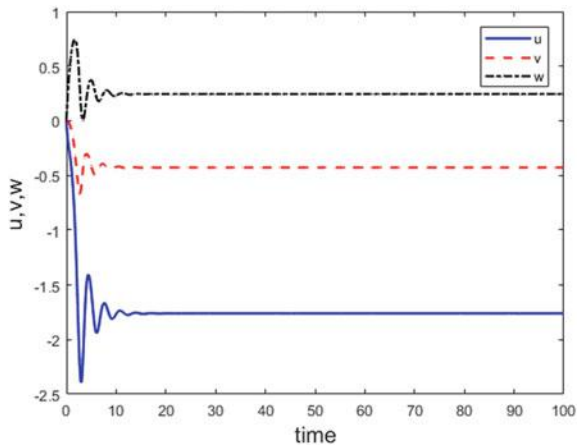
**Fig. 7.22** Three-dimensional parametric plot of system (7.5.2) for  $\alpha = 0.33$  and  $t = 100$



**Fig. 7.23** Three-dimensional parametric plot of system (7.5.2) for  $\alpha = 0.55$  and  $t = 100$

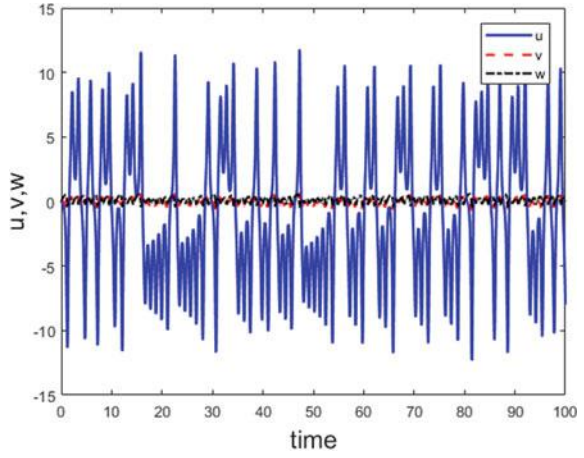


**Fig. 7.24** Time-series plot of system (7.5.2) for  $\alpha = 0.33$  and  $t = 100$

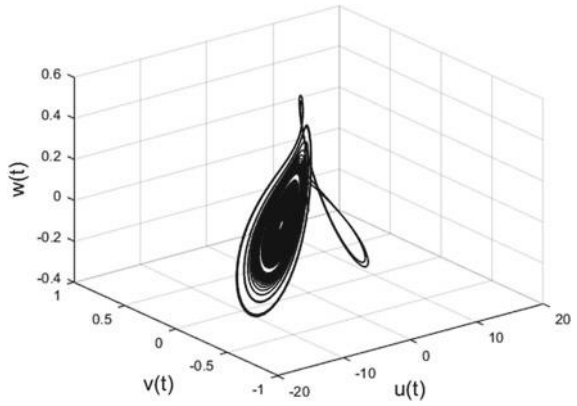


The numerical simulation results for the Caputo time-fractional system (7.5.2) obtained for different values of  $\alpha$  are displayed in Figs. 7.18, 7.19, 7.20, 7.21, 7.22, 7.23, 7.24 and 7.25 which are given in terms of two-dimensional, three-dimensional parametric plots and time-series representation of the system solutions. The approximate solution of chaotic system (7.5.3) using the Caputo–Fabrizio derivative is depicted in Figs. 7.26, 7.27, 7.28, 7.29, 7.30, 7.31, 7.32, 7.33, 7.34, 7.35, 7.36, 7.37 and 7.38. The 2D and 3D representations are displayed in Figs. 7.27, 7.28, 7.29, 7.33, 7.34, 7.35 and 7.26, 7.32, 7.36, 7.37, respectively, while Figs. 7.30, 7.31 and 7.38 correspond to the solution as a function of time  $t$  and different instances of  $\alpha$ .

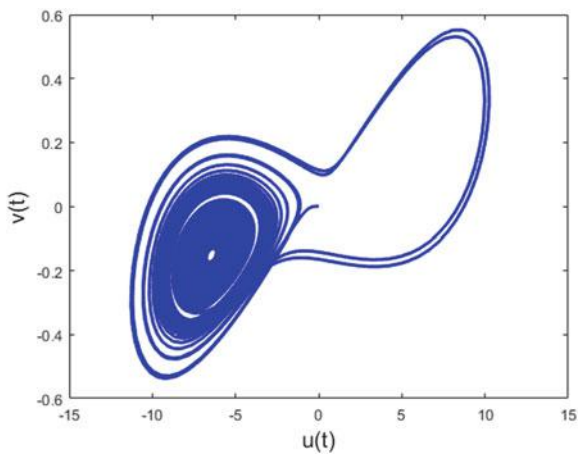
**Fig. 7.25** Time-series plot of system (7.5.2) for  $\alpha = 0.89$  and  $t = 100$



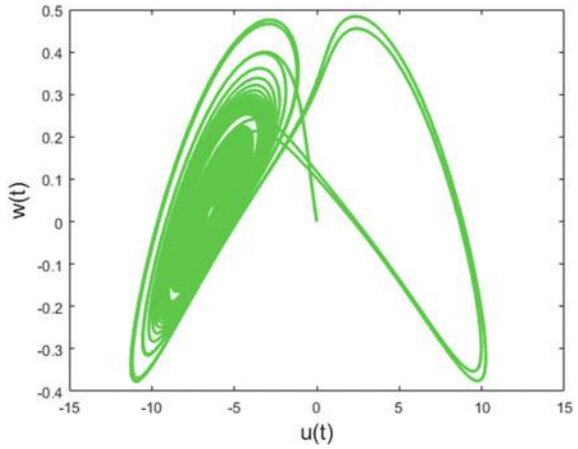
**Fig. 7.26** Three-dimensional representation of chaotic system (7.5.3) for  $\alpha = 0.89$  and  $t = 100$



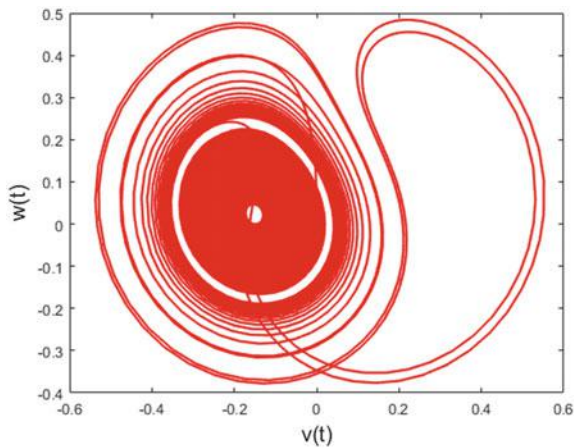
**Fig. 7.27** Two-dimensional plot of  $u(t)$  and  $v(t)$  of chaotic system (7.5.3) for  $\alpha = 0.89$  and  $t = 100$



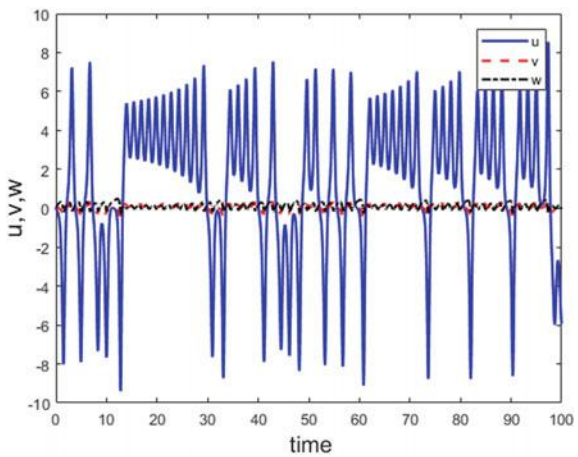
**Fig. 7.28** Two-dimensional plot of  $u(t)$  and  $w(t)$  of chaotic system (7.5.3) for  $\alpha = 0.89$  and  $t = 100$



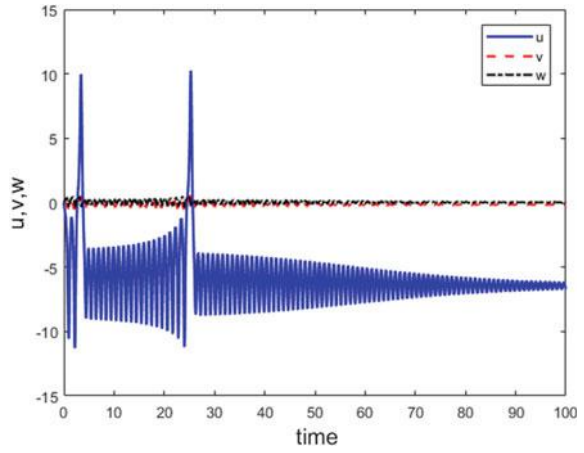
**Fig. 7.29** Two-dimensional plot of  $v(t)$  and  $w(t)$  of chaotic system (7.5.3) for  $\alpha = 0.89$  and  $t = 100$



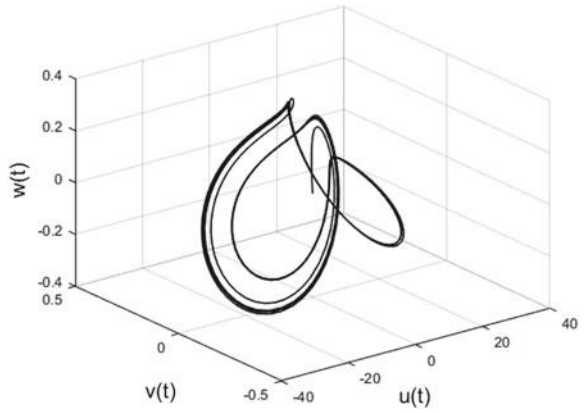
**Fig. 7.30** Solution as a function of time  $t = 100$  for (7.5.3) at  $\alpha = 0.55$



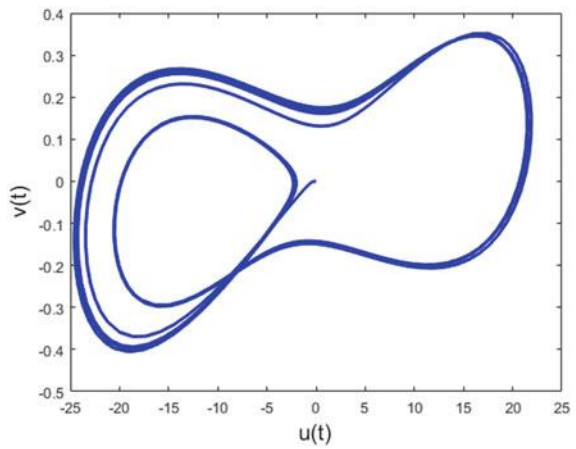
**Fig. 7.31** Solution as a function of time  $t = 100$  for (7.5.3) at  $\alpha = 0.89$



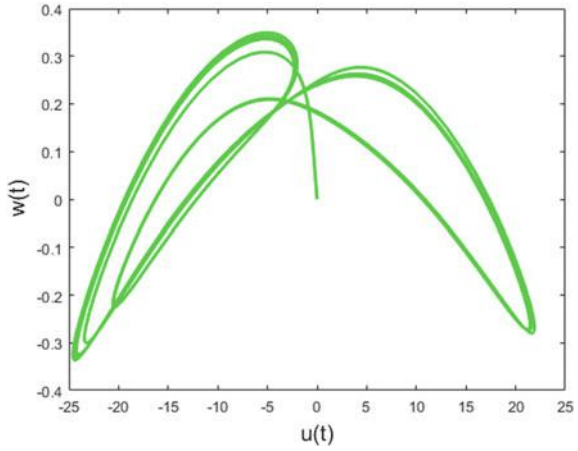
**Fig. 7.32** Three-dimensional representation of chaotic system (7.5.3) for  $\alpha = 0.45$  and  $t = 100$



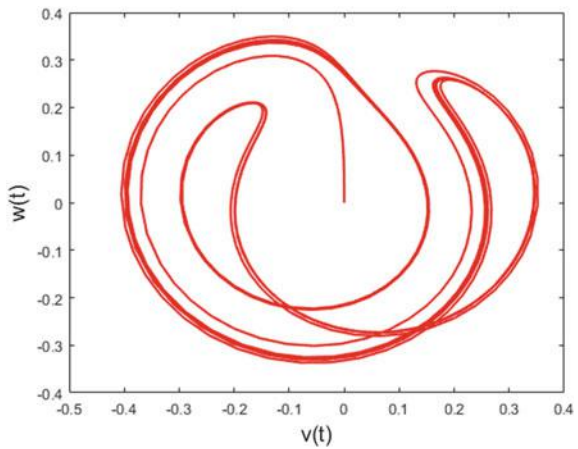
**Fig. 7.33** Two-dimensional plot of  $u(t)$  and  $v(t)$  of chaotic system (7.5.3) for  $\alpha = 0.45$  and  $t = 100$



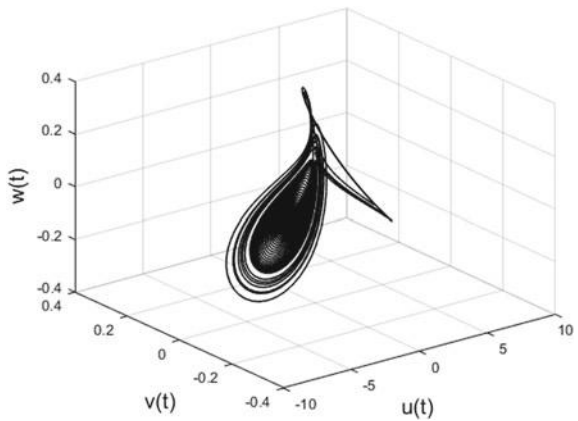
**Fig. 7.34** Two-dimensional plot of  $u(t)$  and  $w(t)$  of chaotic system (7.5.3) for  $\alpha = 0.45$  and  $t = 100$



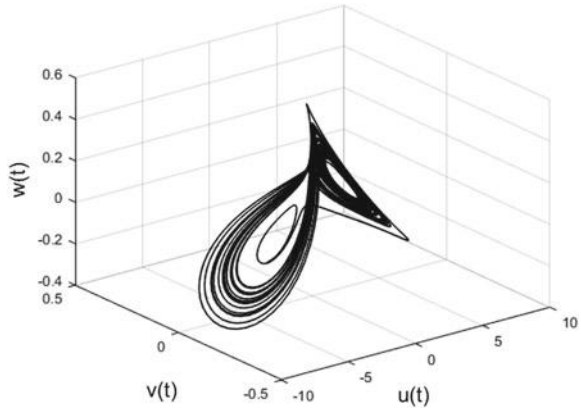
**Fig. 7.35** Two-dimensional plot of  $v(t)$  and  $w(t)$  of chaotic system (7.5.3) for  $\alpha = 0.45$  and  $t = 100$



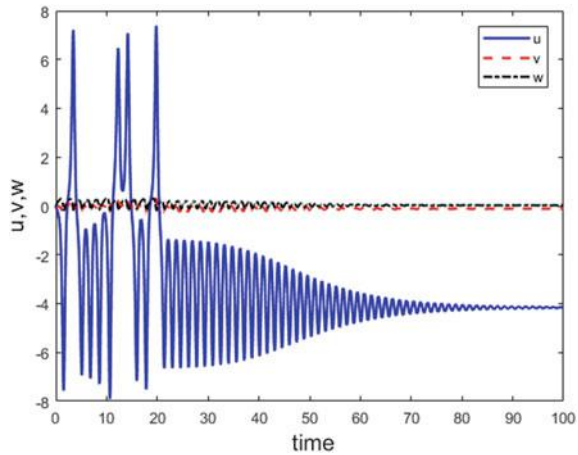
**Fig. 7.36** Three-dimensional representation showing the attraction of system (7.5.3) for  $\alpha = 0.50$  and  $t = 100$



**Fig. 7.37** Three-dimensional representation showing the attraction of system (7.5.3) for  $\alpha = 0.55$  and  $t = 100$



**Fig. 7.38** Solution as a function of time  $t = 100$  for (7.5.3) at  $\alpha = 0.55$  and  $\kappa = 0.50$



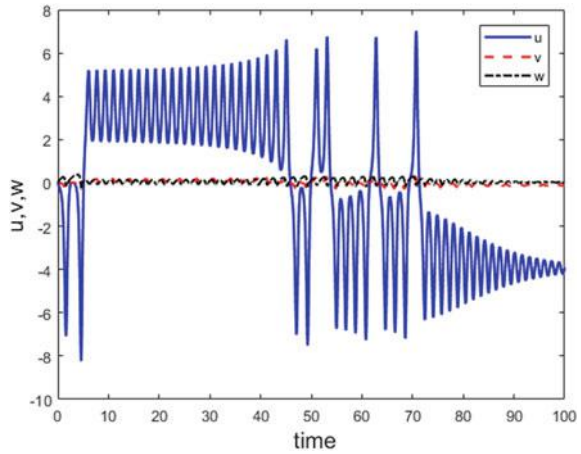
The last experiment on El Niño chaotic system (7.5.1) is based on modelling with the Atangana–Baleanu fractional derivative in the sense of Caputo in the form

$$\begin{aligned}
 {}_0^{ABC}D_t^\alpha u(t) &= \beta v(t) - \gamma u(t) + \gamma \rho, \\
 {}_0^{ABC}D_t^\alpha v(t) &= u(t)w(t) - v(t), \\
 {}_0^{ABC}D_t^\alpha w(t) &= -u(t)v(t) - w(t) + \kappa,
 \end{aligned}
 \tag{7.5.4}$$

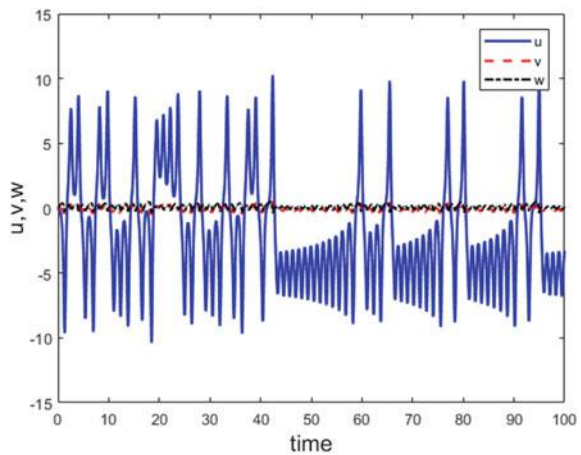
where  ${}_0^{ABC}D_t^\alpha$  is the known Atangana–Baleanu derivative of fractional order  $\alpha \in (0, 1)$ .

Figures 7.39, 7.40, 7.41 and 7.42 depict the time-series solution of (7.5.4) at different instances of  $\alpha$  using the Atangana–Baleanu fractional derivative of order  $0 < \alpha < 1$ . It is observed that all the species undergo spurious and chaotic

**Fig. 7.39** Solution as a function of time  $t = 100$  for (7.5.4) at  $\alpha = 0.45$

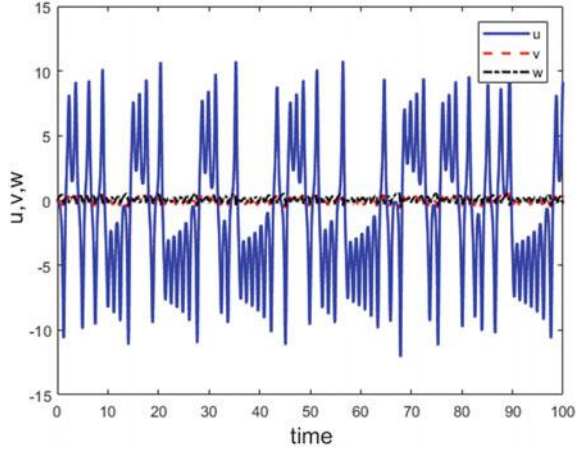


**Fig. 7.40** Solution as a function of time  $t = 100$  for (7.5.4) at  $\alpha = 0.75$

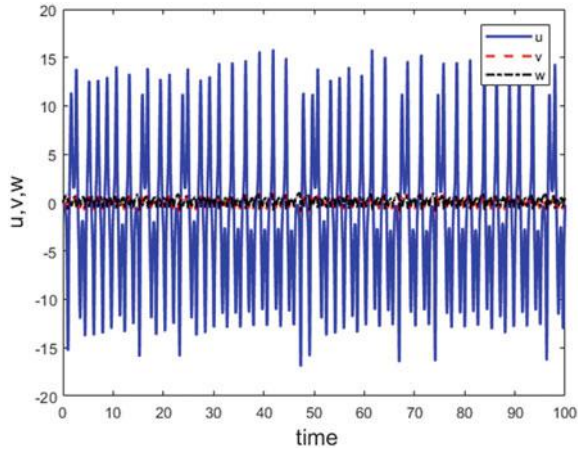


oscillations. At a value close to unity (as  $\alpha \rightarrow 1$ ), if simulation time is reduced, one obtains a smooth or spatiotemporal oscillations and this is evident in Fig. 7.42. The two-, three-dimensional parametric plots using the Atangana–Baleanu derivative in Caputo sense for  $\alpha = 0.35$  and  $\alpha = 0.91$  are displayed in Figs. 7.43, 7.44, 7.45, 7.46 and 7.47, 7.48, 7.49, 7.50, respectively. A close comparison will show the variation in the propagation of models with the Caputo, Caputo–Fabrizio and Atangana–Baleanu derivatives.

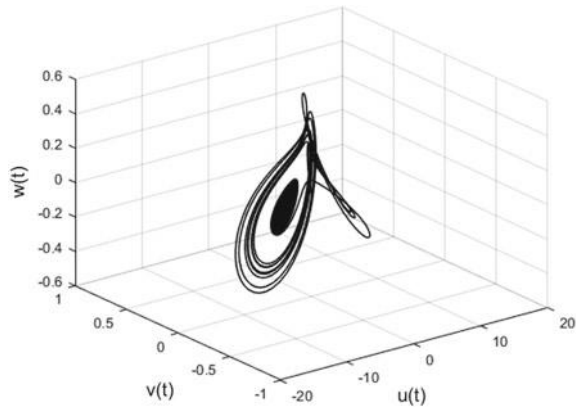
**Fig. 7.41** Solution as a function of time  $t = 100$  for (7.5.4) at  $\alpha = 0.89$



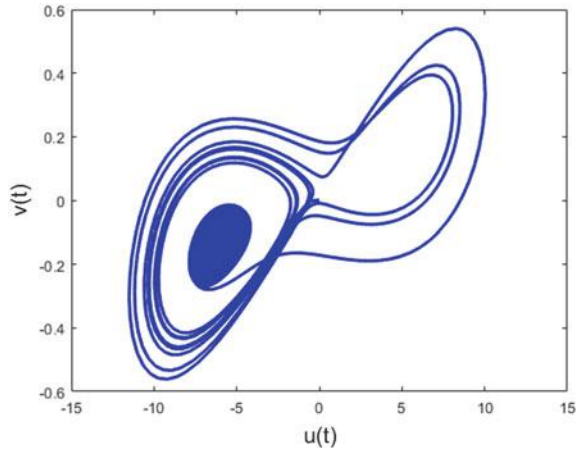
**Fig. 7.42** Solution as a function of time  $t = 100$  for (7.5.4) at  $\alpha = 0.95$



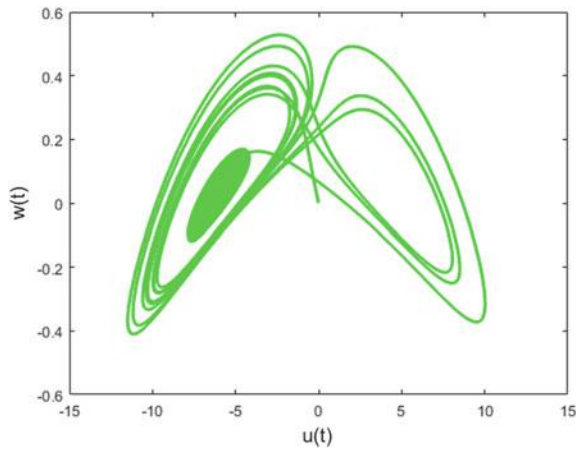
**Fig. 7.43** Three-dimensional representation showing the attraction of system (7.5.4) for  $\alpha = 0.35$  and  $t = 100$



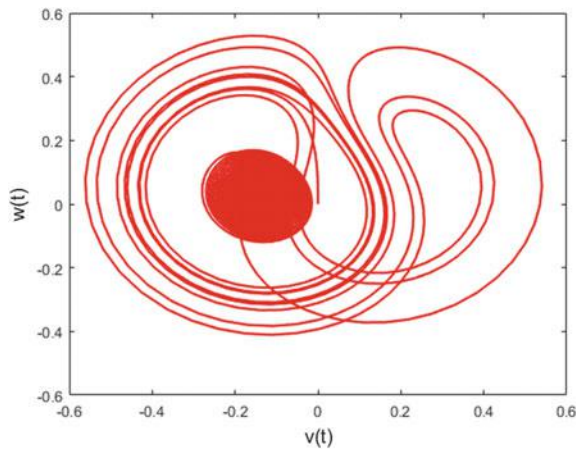
**Fig. 7.44** The two-dimensional representation of system (7.5.4) of  $u(t)$  and  $v(t)$  for  $\alpha = 0.35$  and  $t = 100$



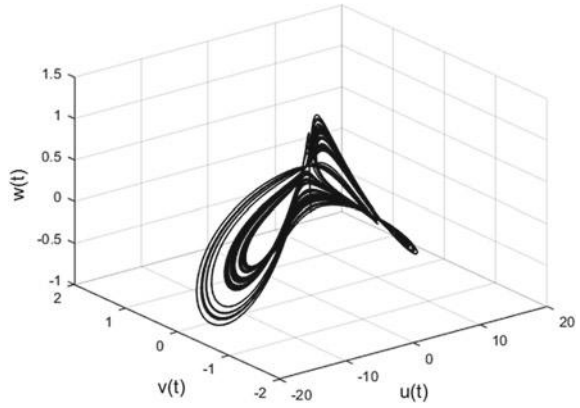
**Fig. 7.45** The two-dimensional representation of system (7.5.4) of  $u(t)$  and  $w(t)$  for  $\alpha = 0.35$  and  $t = 100$



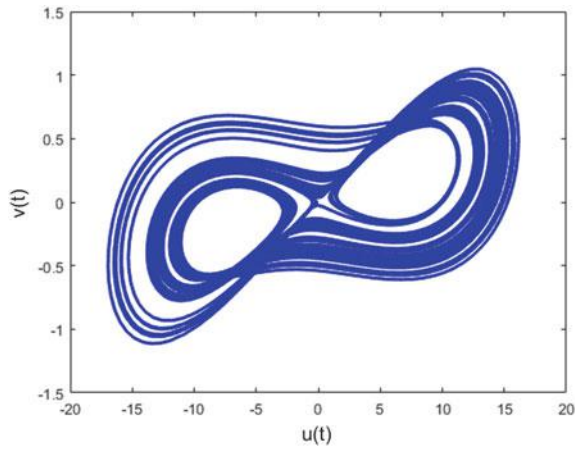
**Fig. 7.46** The two-dimensional representation of system (7.5.4) of  $v(t)$  and  $w(t)$  for  $\alpha = 0.35$  and  $t = 100$



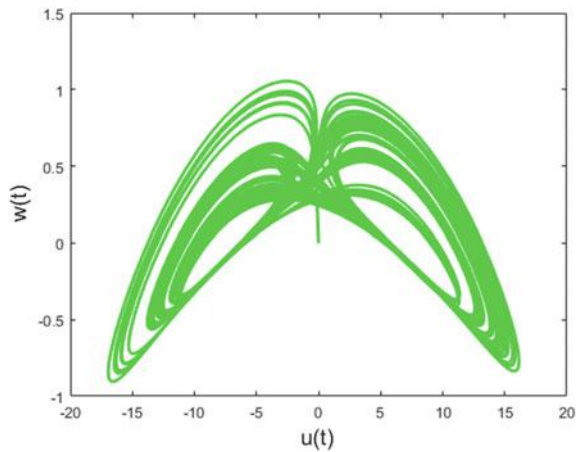
**Fig. 7.47** Three-dimensional representation showing the attraction of system (7.5.4) for  $\alpha = 0.91$  and  $t = 100$



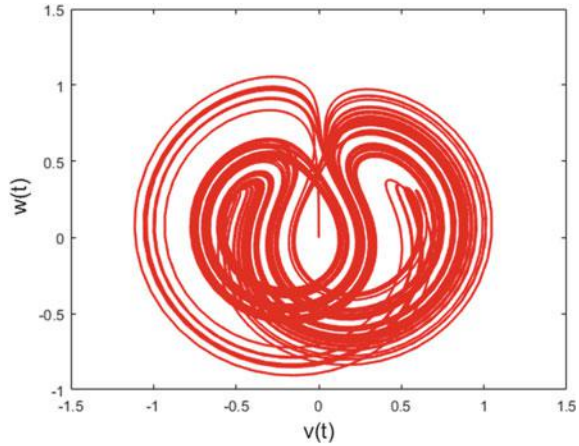
**Fig. 7.48** The two-dimensional representation of system (7.5.4) of  $u(t)$  and  $v(t)$  for  $\alpha = 0.91$  and  $t = 100$



**Fig. 7.49** The two-dimensional representation of system (7.5.4) of  $u(t)$  and  $w(t)$  for  $\alpha = 0.91$  and  $t = 100$



**Fig. 7.50** The two-dimensional representation of system (7.5.4) of  $v(t)$  and  $w(t)$  for  $\alpha = 0.91$  and  $t = 100$



### 7.6 A Novel Fractional Model for the Lassa Hemorrhagic Fever

The lassa hemorrhagic fever is grouped in the family of viridae virus. Its the second largest epidemic outbreak witnessed recently in some part of West Africa and Central Africa countries. Its first emergence was observed in 1969 is Lassa town, situated in Borno State, Nigeria. The main host of this virus is called the Natal multimammate mouse, an animal largely found in most of sub-Saharan Africa countries.

The contamination in human mainly takes place by disclosure to animal excrement through the gastrointestinal or respiratory tracts. Mouthful of air of tiny particle of infective material is known to be the mainly noteworthy way of making contact. It is often likely to get hold of the infection via broken skin or mucous membrane that is in direct contact with the infected material [4].

A research study output has shown that about 15–20% of the patients infected with Lassa fever will die from the disease. However, during epidemic outbreaks, mortality can rise as high as 50% [21]. The death rate is greater than 80% when it occurs among pregnant women usually during their third trimester; according to report in [21], fatal death also recorded in nearly all those cases recorded. We are aiming to give a clear description of the virus spread, infection and mortality rate of the populations of the infected pregnant women.

The mathematical equation underpinning the change in time of the susceptible individual population within the scope of the  $\alpha$ -derivative is defined as

$${}^A_0\mathcal{D}_t^\alpha S(t) = -cS(t)I(t) + bN - \delta N + fR(t) + hS(t) - \delta S(t). \tag{7.6.1}$$

Atangana [4] expressed the change of infected class with an ODE as

$${}^A_0\mathcal{D}_t^\alpha I(t) = cS(t)I(t) - (f + h)I(t) - hS(t). \tag{7.6.2}$$

According to [4], the physical interpretation of Eq.(7.6.2) is that the number of women who are removed from the susceptible population can be expressed as  $cS(t)I(t)$ . However, it was suggested that due to the introduction of medication and vaccines, a number of pregnant women will be recovered at a proportional rate  $h$ , and likewise, the mortality rate of a number of pregnant women will occur at  $f$ . Hence, the change in time of the recovery class is given by

$${}^A_0\mathcal{D}_t^\alpha R(t) = hI(t) - fR(t). \tag{7.6.3}$$

Finally, change in time for the death population is denoted as

$${}^A_0\mathcal{D}_t^\alpha D(t) = fI(t) + \delta N - bN. \tag{7.6.4}$$

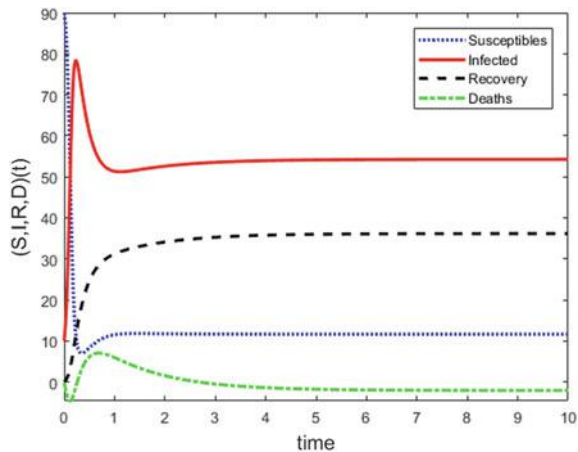
The mathematical equation governing the spread of Lassa fever among pregnant women is given as

$$\begin{aligned} {}^A_0\mathcal{D}_t^\alpha S(t) &= -cS(t)I(t) + bN - \delta N + fR(t) - \delta S(t) + hS(t), \\ {}^A_0\mathcal{D}_t^\alpha I(t) &= cS(t)I(t) - (f + h)I(t) - hS(t), \\ {}^A_0\mathcal{D}_t^\alpha R(t) &= hI(t) - fR(t), \\ {}^A_0\mathcal{D}_t^\alpha D(t) &= fI(t) + IN - bN + \delta S(t), \end{aligned} \tag{7.6.5}$$

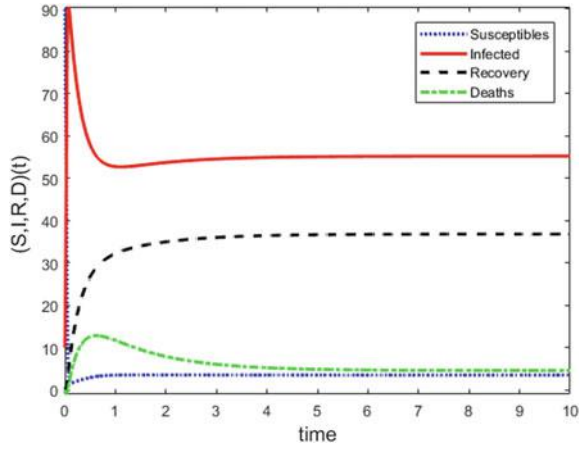
where  $c$  denotes the infections rate,  $h$  is rate at which the pregnant women from recovery class turn out to be vulnerable,  $b$  represents the proportion at which women are pregnant and the mortality rate of pregnant women due to natural death and other outbreaks is represented by  $\delta$ .

For the simulation, the parameters and theoretical values are given as  $N = 1000$ ,  $\delta = 0.2$ ,  $b = 0.3$ ,  $f = 0.8$ ,  $h = 0.2$ ,  $c = 0.4$ ,  $S(0) = 900$ ,  $I(0) = 10$ ,  $R(0) = 0$  and  $D(0) = 0$ . Figures 7.51, 7.52, 7.53 and 7.54 show the future prediction for fractional

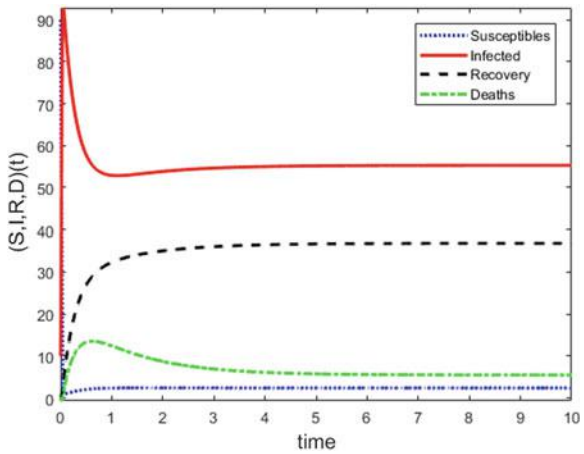
**Fig. 7.51** Prediction for system (7.6.5) when  $\alpha = 0.25$



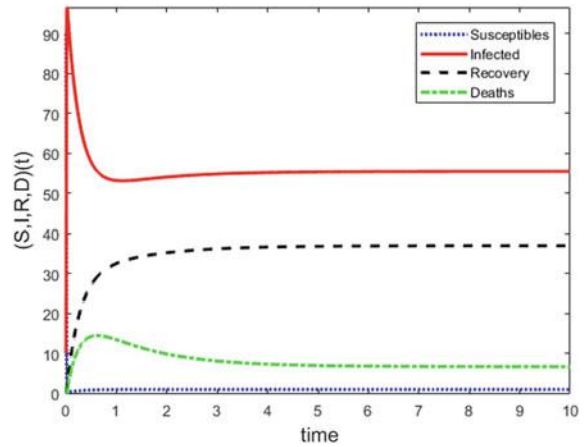
**Fig. 7.52** Prediction for system (7.6.5) when  $\alpha = 0.45$



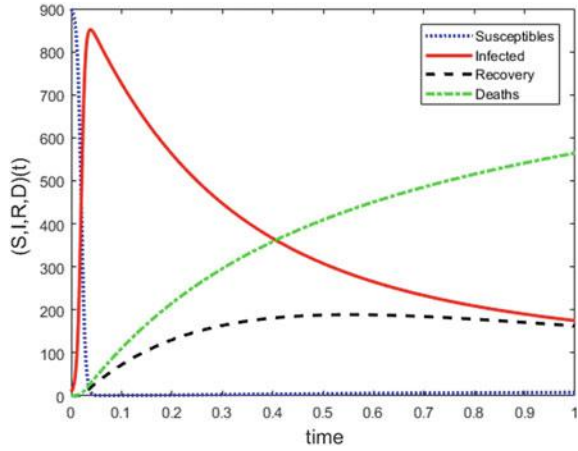
**Fig. 7.53** Prediction for system (7.6.5) when  $\alpha = 0.65$



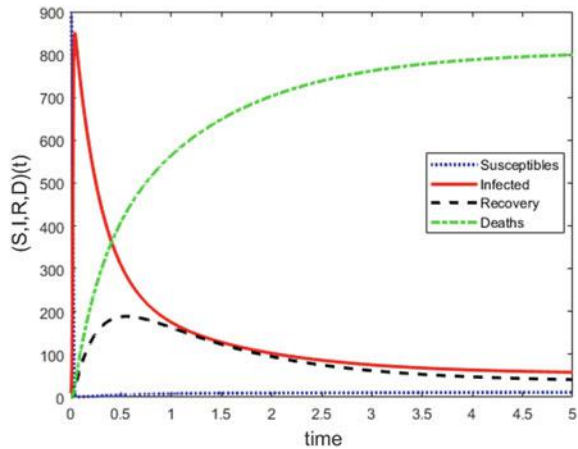
**Fig. 7.54** Prediction for system (7.6.5) when  $\alpha = 0.88$



**Fig. 7.55** Prediction as a function of time  $t = 1.0$  for system (7.6.5) with  $\alpha = 0.50$



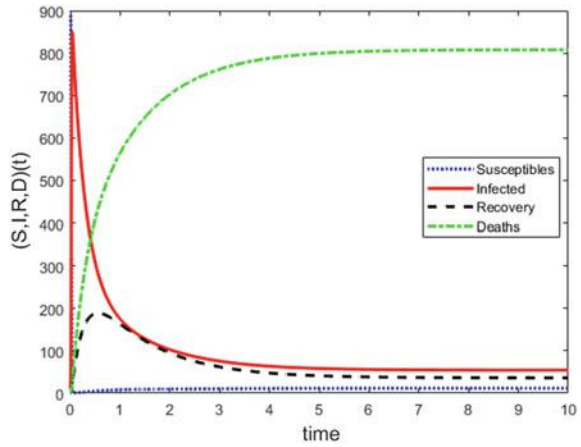
**Fig. 7.56** Prediction as a function of time  $t = 5$  for system (7.6.5) with  $\alpha = 0.50$



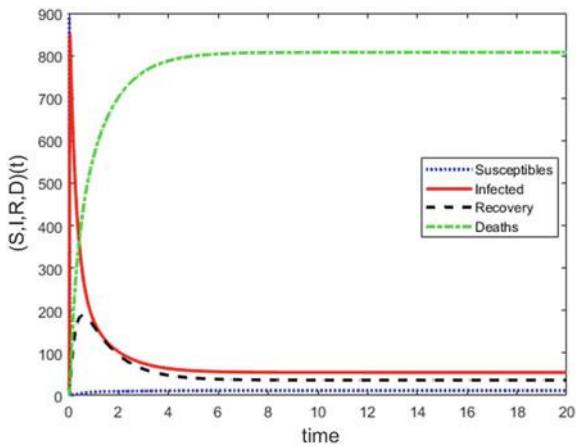
Lassa fever model (7.6.5) for different values of  $\alpha = 0.25, \alpha = 0.45, \alpha = 0.65$  and  $\alpha = 0.88$ , respectively. It is observed that the number of susceptible individuals is reducing as the value of  $\alpha$  is increasing.

In Figs. 7.55, 7.56, 7.57 and 7.58, we present the future prediction of (7.6.5) as a function of different instances of time  $t = 1, 5, 10, 10$ . We observed that if necessary measure is not put in place with the prevalence of the Lassa fever outbreaks, the virus spreads faster with increasing time. Lastly, in Figs. 7.59, 7.60 and 7.61, the effects of  $f$  at  $\alpha = 0.38$  and  $t = 2.0$  which correspond to the mortality rate of pregnant women are examined.

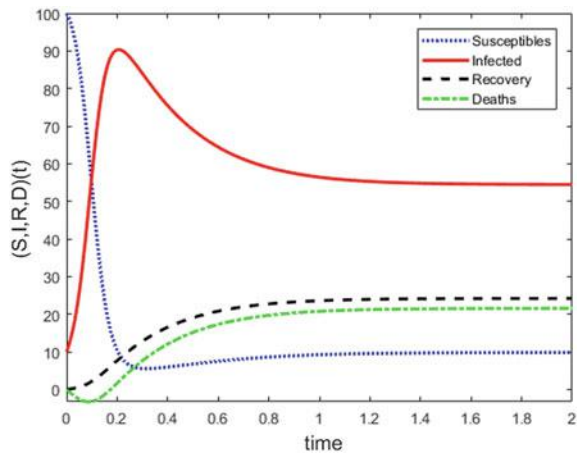
**Fig. 7.57** Prediction as a function of time  $t = 10$  for system (7.6.5) with  $\alpha = 0.50$



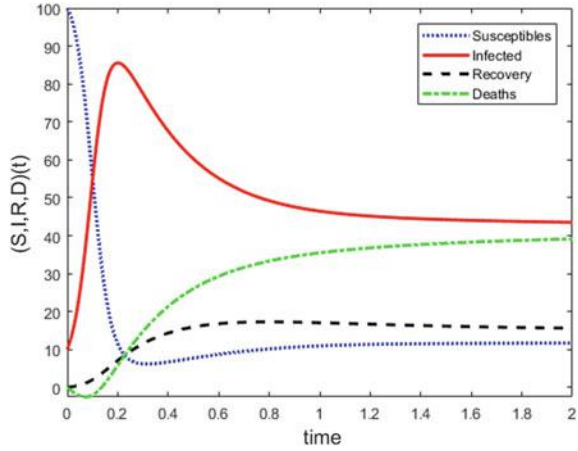
**Fig. 7.58** Prediction as a function of time  $t = 20$  for system (7.6.5) with  $\alpha = 0.50$



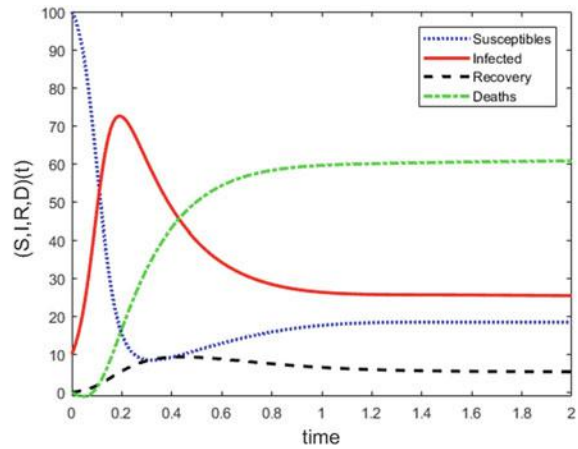
**Fig. 7.59** Future prediction for system (7.6.5) for  $f = 1.8$



**Fig. 7.60** Future prediction for system (7.6.5) for  $f = 2.28$



**Fig. 7.61** Future prediction for system (7.6.5) for  $f = 3.28$



### 7.7 Modelling of Ebola Hemorrhagic Fever: Fractional Derivative Approach

Known that the filoviruses comes from a virus family called Filoviridae. This virus may cause unembellished hemorrhagic fever in both humans and monkeys [13, 16, 17]. In most research papers and monographs, only two classes of this virus family have been identified so far, they are, Ebola virus and Marburg virus. Also, according to the literature, only five species of Ebola virus have been distinguished including Bundibugyo, Ivory Coast, Sudan, Zaire and Reston. Among these species, Ebola virus is known to be the only family of the Zaire Ebola virus species and the most dangerous and largest recorded epidemic outbreaks [3, 17].

Ebola is an uncommon but dangerous virus that results in bleeding inside and outside of the body [11]. As the virus spreads through the body, it breaks down the

immune system and organs. Ultimately, it drops the levels of blood clotting in the cells [1]. This results in severe and uncontrollable bleeding [11, 17]. The biggest challenge in most West African nations is issue of unemployment. Findings have revealed that about 133 million working class people which constitute about 50% of the population are illiterate and jobless. Many of these young people lack economic or social life skills which completely render them useless in the labour market. As a means to survive and provide minimum basic needs for their family, the only available jobs include fishing, farming and hunting.

In the case of hunting and destruction of ecosystem, many of the wild animals are killed and endangered, the practice majority do routinely to survive. Most of the animals killed are either consumed fresh or dry and sold in the market places. Incidentally, it is a common belief that the Ebola virus disease can only occur after an Ebola virus is transmitted to an initial human by contact with an infected animal's body fluid. On contrary, human-to-human transmission when direct contact is made to the bodily fluid or blood of the infected person. Fruit bats are known to be the most likely natural source of the Ebola virus. As the early transmission, the bat drops incompletely eaten fruits and pulp, and when it lands animals such as monkeys and gorillas feed on fallen fruits. Later, the humans hunt down these animals as food or sell the infected animal bodies to make money. Definitely the affected human will make contact with the rest of his family. So, the chain of transmission continues.

For the mathematical formulation, we let  $S(t)$ ,  $I(t)$ ,  $R(t)$  and  $D(t)$  be the respective susceptible, infected, recovery and the total mortality or death populations. Likewise, let  $s$ ,  $i$ ,  $r$  and  $\delta$  be the susceptibility rate, infection rate, recovery rate and death rate by Ebola. The mathematical model describing the rate of change of susceptible individuals is represented as

$$\frac{dS(t)}{dt} = -iS(t)I(t) + sR(t) - \beta N, \quad (7.7.1)$$

where  $i$  describes the rate of infectious class from recovery individuals converted to be vulnerable at rate  $s$ , and  $\beta$  denote the number of population that die naturally due to other diseases.

The rate of change of infected population is given by the differential equation

$$\frac{dI(t)}{dt} = -iS(t)I(t) - \delta I(t) - rI(t), \quad (7.7.2)$$

which suggests that the total number of individuals removed from susceptible class can be expressed mathematically as  $iS(t)I(t)$ . Obviously, due to medication, a reasonable number of populations will be recovered at rate  $r$ , while infected individual will die at rate  $\delta$ . The recovery population and the change in mortality rate can be described by the following respective ordinary differential equations:

$$\frac{dR(t)}{dt} = rI(t) - sR(t) \quad (7.7.3)$$

and

$$\frac{dD(t)}{dt} = \delta I(t) + \beta N. \tag{7.7.4}$$

Thus, the mathematical equation governing the Ebola virus disease is given as

$$\begin{aligned} \frac{dS(t)}{dt} &= -iS(t)I(t) + s(t) - \delta N, \\ \frac{dI(t)}{dt} &= iS(t)I(t) - \delta I(t) - rI(t), \\ \frac{dR(t)}{dt} &= rI(t) - sR(t), \\ \frac{dD(t)}{dt} &= \delta I(t) + \beta N. \end{aligned} \tag{7.7.5}$$

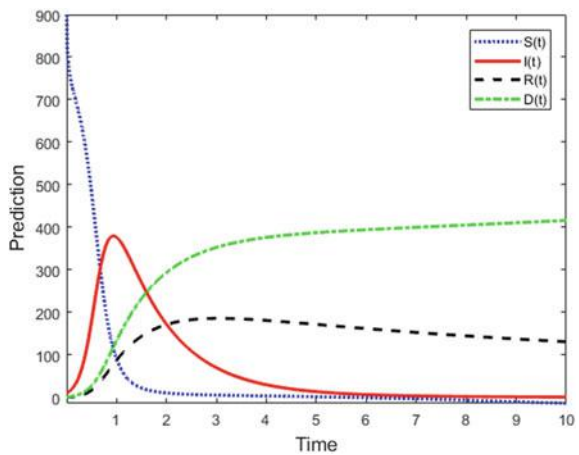
The above equation will be formulated in terms of the Caputo–Fabrizio and the Atangana–Baleanu fractional derivatives, respectively, as

$$\begin{aligned} {}_0^C\mathcal{D}_t^\alpha S(t) &= -iS(t)I(t) + s(t) - \delta N, \\ {}_0^C\mathcal{D}_t^\alpha I(t) &= iS(t)I(t) - \delta I(t) - rI(t), \\ {}_0^C\mathcal{D}_t^\alpha R(t) &= rI(t) - sR(t), \\ {}_0^C\mathcal{D}_t^\alpha D(t) &= \delta I(t) + \beta N, \end{aligned} \tag{7.7.6}$$

**Table 7.2** Parameters based on some reported data

Parameters	$S(0)$	$I(0)$	$R(0)$	$D(0)$	$N$	$\beta$	$r$	$i$	$s$	$\delta$
Values	900	10	0	0	1000	0.01	0.4	0.01	0.02	0.6

**Fig. 7.62** Prediction of the Caputo–Fabrizio fractional derivative model (7.7.6) for  $\alpha = 0.25$



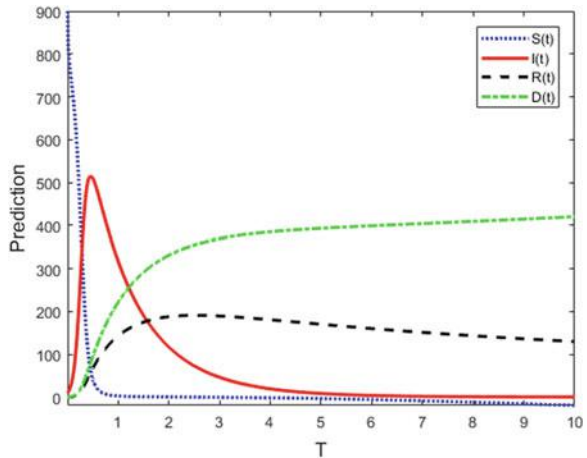
and

$$\begin{aligned}
 {}_0^{ABC}D_t^\alpha S(t) &= -iS(t)I(t) + s(t) - \delta N, \\
 {}_0^{ABC}D_t^\alpha I(t) &= iS(t)I(t) - \delta I(t) - rI(t), \\
 {}_0^{ABC}D_t^\alpha R(t) &= rI(t) - sR(t), \\
 {}_0^{ABC}D_t^\alpha D(t) &= \delta I(t) + \beta N.
 \end{aligned}
 \tag{7.7.7}$$

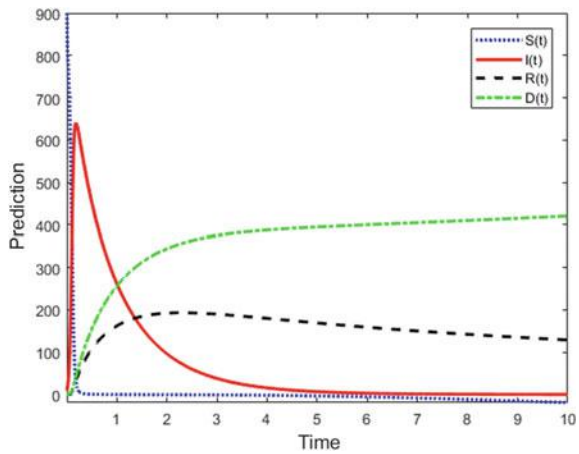
The parameters used for the numerical simulations according to reported data are given in Table 7.2.

Figures 7.62, 7.63, 7.64, 7.65 and 7.66 depict the approximate solution of the Caputo–Fabrizio time-fractional Ebola system (7.7.6) for different values of  $\alpha$  as shown in the figures’ captions. Figures 7.67, 7.68, 7.69, 7.70, 7.71 and 7.72 represent

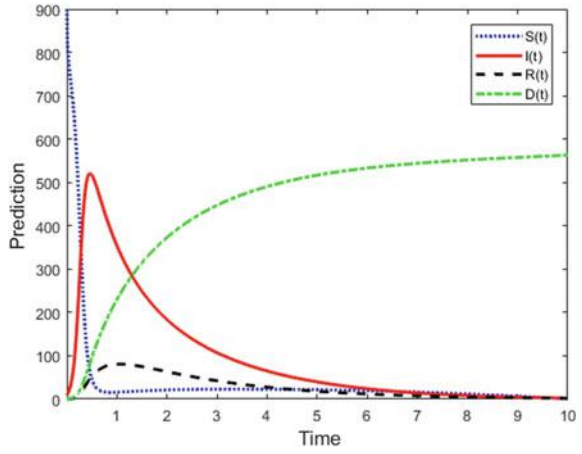
**Fig. 7.63** Prediction of the Caputo–Fabrizio fractional derivative model (7.7.6) for  $\alpha = 0.45$



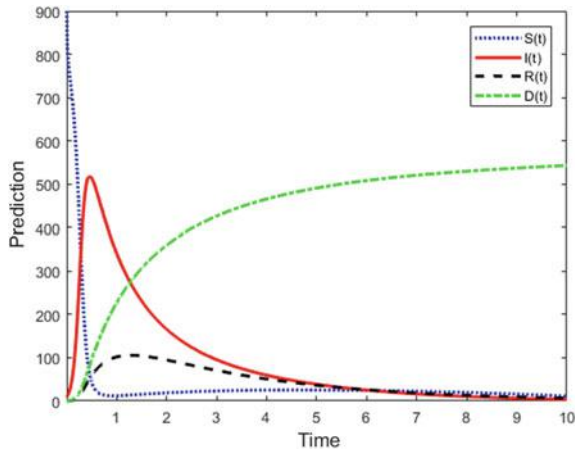
**Fig. 7.64** Prediction of the Caputo–Fabrizio fractional derivative model (7.7.6) for  $\alpha = 0.67$



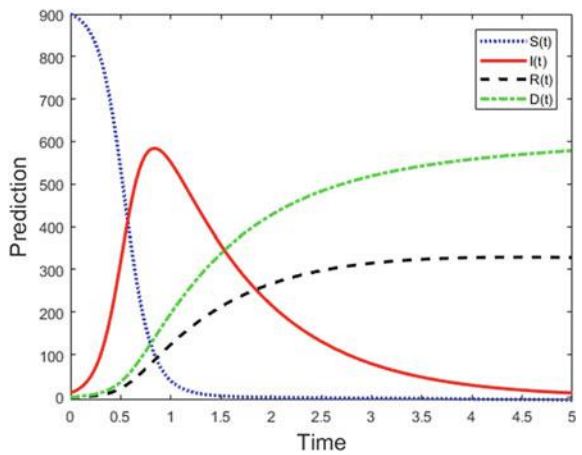
**Fig. 7.65** Prediction of the Caputo–Fabrizio fractional derivative model (7.7.6) for  $\alpha = 0.83$



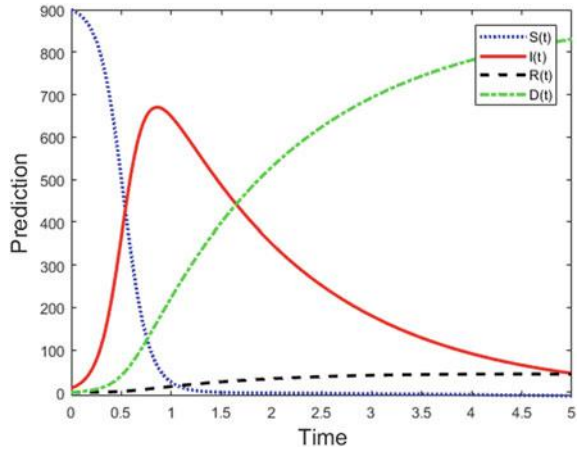
**Fig. 7.66** Prediction of the Caputo–Fabrizio fractional derivative model (7.7.6) for  $\alpha = 0.90$



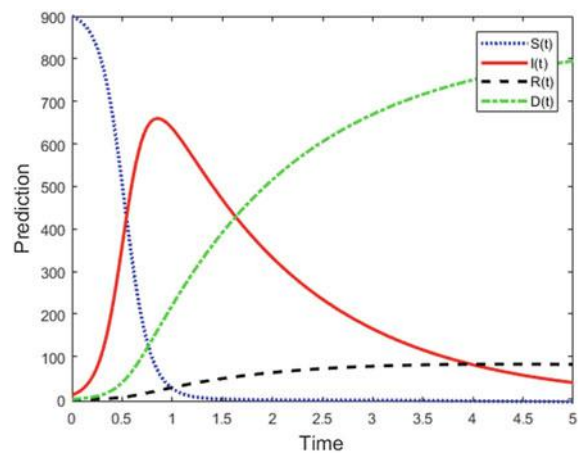
**Fig. 7.67** Prediction using the Atangana–Baleanu fractional derivative model (7.7.7) for  $\alpha = 0.25$



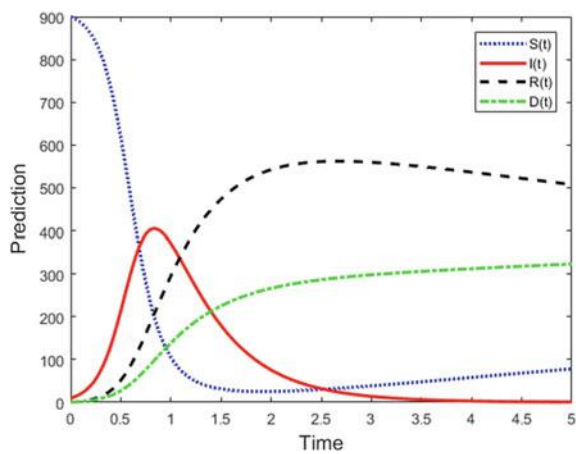
**Fig. 7.68** Prediction using the Atangana–Baleanu fractional derivative model (7.7.7) for  $\alpha = 0.55$



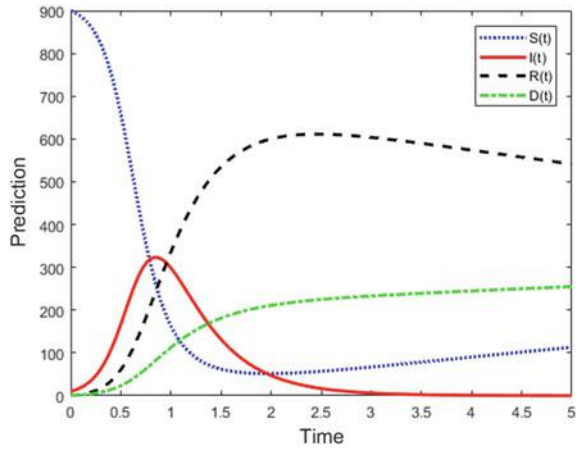
**Fig. 7.69** Prediction using the Atangana–Baleanu fractional derivative model (7.7.7) for  $\alpha = 0.59$



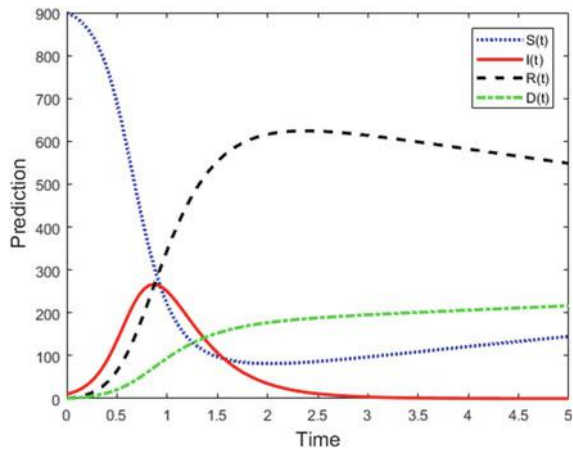
**Fig. 7.70** Prediction using the Atangana–Baleanu fractional derivative model (7.7.7) for  $\alpha = 0.83$



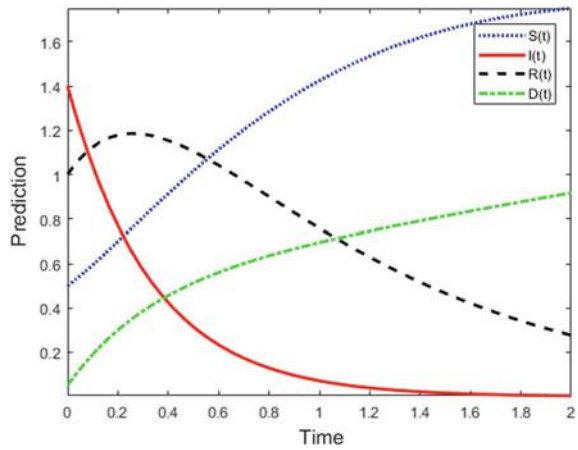
**Fig. 7.71** Prediction using the Atangana–Baleanu fractional derivative model (7.7.7) for  $\alpha = 0.89$



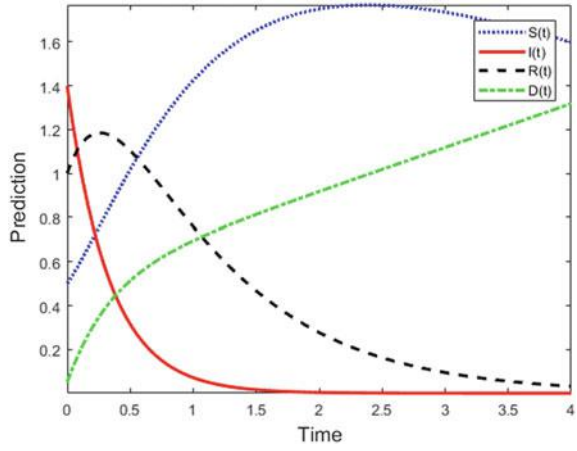
**Fig. 7.72** Prediction using the Atangana–Baleanu fractional derivative model (7.7.7) for  $\alpha = 0.93$



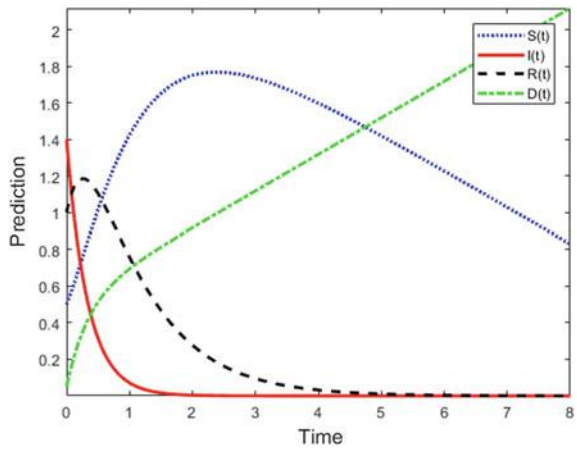
**Fig. 7.73** Prediction for system (7.7.7) at  $t = 2$



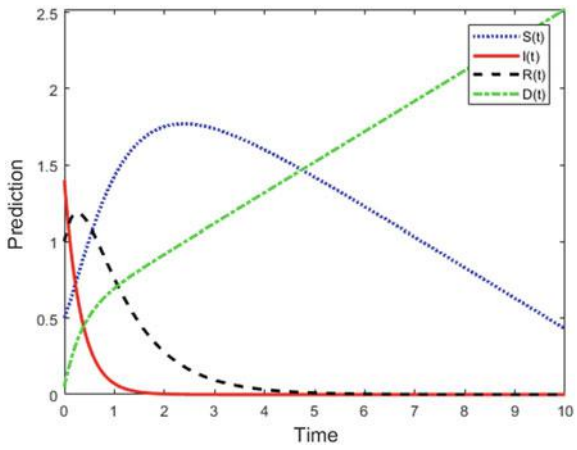
**Fig. 7.74** Prediction for system (7.7.7) at  $t = 4$



**Fig. 7.75** Prediction for system (7.7.7) at  $t = 8$



**Fig. 7.76** Prediction for system (7.7.7) at  $t = 10$



the approximate numerical solution of the Atangana–Baleanu fractional derivative system (7.7.7) for different instances of  $\alpha$  as displayed in the figures' captions. Finally, we fixed  $\alpha = 0.50$  with perturbed initial conditions to examine the effect of time as given in Figs. 7.73, 7.74, 7.75 and 7.76.

## References

1. J. Al-Omari, S.A. Gourley, Monotone travelling fronts in an age-structured reaction-diffusion model of a single species. *J. Math. Biol.* **45**, 294–312 (2002)
2. A. Atangana, R.T. Alqahtani, Modelling the spread of river blindness disease via the Caputo fractional derivative and the beta-derivative. *Entropy* **18**, 40 (2018). <https://doi.org/10.3390/e18020040>
3. A. Atangana, E.F. Doungmo Goufo, On the mathematical analysis of Ebola hemorrhagic fever: deathly infection disease in West African countries. *BioMed Res. Int.* Article ID 261383, 7 pages (2014). <https://doi.org/10.1155/2014/261383>
4. A. Atangana, A novel model for the lassa hemorrhagic fever: deathly disease for pregnant women. *Neural Comput. Appl.* **26**, 1895–1903 (2015)
5. A. Atangana, *Derivative with a New Parameter: Theory, Methods and Applications* (Academic Press, New York, 2016)
6. A. Atangana, *Fractional Operators With Constant and Variable Order with Application to Geo-Hydrology* (Academic Press, New York, 2017)
7. J. Cao, C. Xu, A high order schema for the numerical solution of the fractional ordinary differential equations. *J. Comput. Phys.* **238**, 154–168 (2013)
8. M. Caputo, Linear models of dissipation whose  $Q$  is almost frequency independent II. *Geophys. J. R. Astron. Soc.* **13**, 529–539 (1967)
9. M. Caputo, M. Fabrizio, A new definition of fractional derivative without singular kernel. *Prog. Fract. Differ. Appl.* **1**, 73–85 (2015)
10. G. Gao, H. Sun, Three-point combined compact alternating direction implicit difference schemes for two-dimensional time-fractional advection-diffusion equations. *Commun. Comput. Phys.* **17**, 487–509 (2017)
11. T. Hoenen, A. Groseth, D. Falzarano, H. Feldmann, Ebola virus: unravelling pathogenesis to combat a deadly disease. *Trends Mol. Med.* **12**, 206–215 (2006)
12. I. Koca, A. Atangana, Analysis of a nonlinear model of interpersonal relationships with time fractional derivative. *J. Math. Anal.* **7**, 1–11 (2016)
13. J.H. Kuhn, S. Becker, H. Ebihara et al., Proposal for a revised taxonomy of the family Filoviridae: classification, names of taxa and viruses, and virus abbreviations. *Arch. Virol.* **155**, 2083–2103 (2010)
14. P. Kumar, O.P. Agrawal, An approximate method for numerical solution of fractional differential equations. *Signal Process* **86**, 2602–2610 (2006). Special Section: Fractional Calculus Applications in Signals and Systems
15. T.A.M. Langlands, B.I. Henry, The accuracy and stability of an implicit solution method for the fractional diffusion equation. *J. Comput. Phys.* **205**, 719–736 (2005)
16. E.K. Leffel, D.S. Reed, Marburg and Ebola viruses as aerosol threats. *Biosecurity Bioterrorism Biodefense Strat. Pract. Sci.* **2**, 186–191 (2004)
17. E. Leroy, J.P. Gonzalez, X. Pourrut, Ebolavirus and other filoviruses. *Curr. Top. Microbiol. Immunol.* **315**, 363–387 (2007)
18. Y. Lin, C. Xu, Finite difference/spectral approximations for the time-fractional diffusion equation. *J. Comput. Phys.* **225**, 1533–1552 (2007)
19. J. Liu, Z. Ma, Z. Zhou, Explicit and implicit TVD schemes for conservation laws with Caputo derivatives. *J. Sci. Comput.* **72**, 291–313 (2017)

20. C. Lv, C. Xu, Improved error estimates of a finite difference/spectral method for time-fractional diffusion equations. *Int. J. Numer. Anal. Model.* **12**, 384–400 (2015)
21. J.B. McCormick, P.A. Webb, J.W. Krebs, K.M. Johnson, E.S. Smith, A prospective study of the epidemiology and ecology of Lassa fever. *J. Infect. Dis.* **155**, 437 (1987)
22. P.R. Murray, *Medical Microbiology*, 7th edn. (Elsevier Saunders, Philadelphia, PA, USA, 2013)
23. N. Ozalp, I. Koca, A fractional order nonlinear dynamical model of interpersonal relationships. *Adv. Differ. Equ.* **189**, 7 pages (2012). <https://doi.org/10.1186/1687-1847-2012-189>
24. J.R.C. Piqueira, V.O. Araujo, A modified epidemiological model for computer viruses. *Appl. Math. Comput.* **2**, 355–360 (2018)
25. S. Samko, A. Kilbas, O. Marichev, *Fractional Integrals and Derivatives: Theory and Applications* (Gordon and Breach, Amsterdam, 1993)
26. S.H. Strogatz, *Nonlinear Dynamics and Chaos: With Applications to Physics, Biology, Chemistry and Engineering* (Addison-Wesley, Reading, MA, 1994)
27. Z. Sun, X. Wu, A fully discrete difference scheme for a diffusion-wave system. *Appl. Numer. Math.* **56**, 193–209 (2006)
28. B. Thylefors, M.M. Alleman, N.A. Twum-Danso, Operational lessons from 20 years of the Mectizan Donation Program for the control of onchocerciasis. *Trop. Med. Int. Health* **13**, 689–696 (2008)
29. C. Wang, J. Liu, Positivity property of second-order flux-splitting schemes for the compressible euler equations. *Discret. Contin. Dyn. Syst. Ser. B* **3**, 201–228 (2003)
30. X. Zhao, Z. Sun, G.E. Karniadakis, Second-order approximations for variable order fractional derivatives: algorithms and applications. *J. Comput. Phys.* **293**, 184–200 (2015)

# Chapter 8

## Application to Partial Fractional Differential Equation



Numerical methods for fractional partial differential equations have also been intensively studied and many already published papers can be found in the literature. Due to their wider application in modelling complex real-world problems, several numerical schemes have been suggested. This chapter is devoted to the discussion underpinning the application of existing and newly established numerical schemes for solving partial fractional differential equations.

### 8.1 Space-Fractional Diffusion Equation with New (Atangana–Gomez) Fractional Derivative in Riemann–Liouville Sense

We wrap up this analysis by studying the possibility of applying the numerical version of the new Riemann–Liouville fractional derivative (3.6.13) discussed in Chap. 3 with no singular kernel to a popular diffusion process. The equation under consideration here is

$$\mathbf{D}_t^\alpha u(x, t) = \frac{\partial^2}{\partial x^2} u(x, t). \quad (8.1.1)$$

For the spatial discretization, we let

$$x_s = s\hbar, \quad (8.1.2)$$

with  $0 \leq s \leq N$ ,  $\hbar$  the step size and  $N$  the grid points. We adapt the following Crank–Nicholson scheme for the second-order derivative about the spatial coordinate:

$$\frac{d^2U}{dx^2} = \frac{U(x_{s+1}, t_k) - 2U(x_s, t_k) + U(x_{s-1}, t_k)}{2\hbar^2} + \mathcal{O}(\hbar^2). \tag{8.1.3}$$

Next, by using Eq. (8.1.3) in (8.1.1), we have

$$\begin{aligned} \frac{M(\alpha)}{\alpha h} & \left[ \sum_{i=1}^{k+1} (u(x_s, t_{i+1}) + u(x_s, t_i)) \chi_{i,h} - \sum_{i=1}^k (u(x_s, t_{i+1}) + u(x_s, t_i)) \bar{\chi}_{i,h} \right] \\ & - \frac{u(x_{s+1}, t_k) - 2u(x_s, t_k) + u(x_{s-1}, t_k)}{\hbar^2} = 0. \end{aligned} \tag{8.1.4}$$

For simplicity, we let  $u_s^i = u(x_s, t_i)$ , then

$$\frac{M(\alpha)}{\alpha h} \left[ \sum_{i=1}^{k+1} (u_s^{i+1} + u_s^i) \chi_{i,h} - \sum_{i=1}^{k+1} (u_s^{i+1} + u_s^i) \bar{\chi}_{i,h} \right] - \frac{u_{s+1}^k - 2u_s^k - u_{s-1}^k}{\hbar^2} = 0. \tag{8.1.5}$$

After rearranging, we obtain

$$\begin{aligned} u_s^{k+1} \left\{ \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h}) \right\} & = u_s^k \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) - \frac{2}{\hbar^2} \right] \\ & - \frac{M(\alpha)}{\alpha h} \left[ \sum_{\substack{i=1 \\ i \neq k}}^{k+1} (u_s^{i+1} + u_s^i) \chi_{i,h} - \sum_{i=1}^{k-1} (u_s^{i+1} + u_s^i) \bar{\chi}_{i,h} \right] \\ & + \frac{u_{s+1}^k + u_{s-1}^k}{\hbar^2}. \end{aligned} \tag{8.1.6}$$

**Stability Analysis**

Also, in this section, we examine the stability conditions of the numerical scheme. Assume  $v_s^i = u_s^i - U_s^i$ , where  $F_s^i$  denotes the approximate solution at the point  $(x_s, t_i)$ ,  $s = 1, 2, \dots, N$ ,  $i = 1, 2, \dots, S$ . Moreover,  $v^i = [v_1^i, v_2^i, \dots, v_{N-1}^i]^T$  and the function  $v^i(x)$  satisfies

$$v^i(x) = \begin{cases} v_s^i(x) & \text{if } x_s - \frac{\hbar}{2} < x < x_s + \frac{\hbar}{2} \\ 0 & \text{if } L - \frac{\hbar}{2} < x < L. \end{cases}$$

Then, we give the error of the numerical scheme when applying to solve the diffusion equation (8.1.1) as

$$\begin{aligned}
v_s^{k+1} \left[ \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h}) \right] &= v_s^k \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) - \frac{2}{h^2} \right] \\
&\quad - \frac{M(\alpha)}{\alpha h} \left[ \sum_{\substack{i=1 \\ i \neq k}}^{k+1} (v_s^{i+1} + v_s^i) \chi_{i,h} - \sum_{i=1}^{k-1} (v_s^{i+1} + v_s^i) \bar{\chi}_{i,h} \right] \\
&\quad + \frac{v_s^k + v_s^{k-1}}{h^2}. \tag{8.1.7}
\end{aligned}$$

Using Fourier series, we can express the function  $v^i(x)$  as

$$v^i(x) = \sum_{m=-\infty}^{m=+\infty} \delta_m(x) \exp[2j\pi mi/L].$$

Hence, in a more explicit form,  $v_s^i(x)$  q(r) can be written in the delta-exponential form as

$$v_s^i = \delta_i \exp[j\zeta i s], \tag{8.1.8}$$

where  $\zeta$  is a real spatial wave number. On substituting (8.1.8) into (8.1.7), we have For  $k = 0$ ,

$$\begin{aligned}
\delta_1 \left[ \frac{M(\alpha)}{\alpha h} (\chi_{0,h} - \bar{\chi}_{0,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right] \\
= \delta_0 \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{0,h} - \chi_{0,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h} \sin^2 \left( \frac{\zeta_i}{2} \right) \right]. \tag{8.1.9}
\end{aligned}$$

For  $k \geq 1$

$$\begin{aligned}
\delta_{k+1} \left[ \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right] &= \delta_k \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h} \sin^2 \left( \frac{\zeta_i}{2} \right) \right] \\
&\quad - \frac{M(\alpha)}{\alpha h} \left[ \sum_{\substack{i=1 \\ i \neq k}}^{k+1} (\delta_{i+1} + \delta_i) \chi_{i,h} - \sum_{i=1}^{k-1} (\delta_{i+1} + \delta_i) \bar{\chi}_{i,h} \right] + \frac{2\delta_k}{h^2}. \tag{8.1.10}
\end{aligned}$$

We rearrange (8.1.10) after some algebraic manipulations to obtain

$$\begin{aligned}
\delta_{k+1} \left[ \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right] &= \delta_k \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h} \sin^2 \left( \frac{\zeta_i}{2} \right) \right] \\
&\quad - \frac{M(\alpha)}{\alpha h} \left[ 2 \sum_{\substack{i=1 \\ i \neq k}}^{k+1} \delta_i \chi_{i,h} - 2 \sum_{i=1}^{k-1} \delta_i \bar{\chi}_{i,h} \right] + \frac{2\delta_k}{h^2}. \tag{8.1.11}
\end{aligned}$$

Now to complete the stability analysis for the new fractional Riemann–Liouville derivative approximation scheme, we require to show that

$$\left| \frac{\delta_k}{\delta_0} \right| \leq 1, \quad \text{for all } k = 0, 1, 2. \tag{8.1.12}$$

Next, we proceed by recurrence.

For  $k = 0$ , Eq. (8.1.10) gives

$$\begin{aligned} \left| \frac{\delta_k}{\delta_0} \right| &= \frac{\left| \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{0,h} - \chi_{0,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h^2} \sin^2 \left( \frac{\zeta_i}{2} \right) \right|}{\left| \frac{M(\alpha)}{\alpha h} (\chi_{0,h} - \bar{\chi}_{0,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right|} \\ &\leq \frac{\left| \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{0,h} - \chi_{0,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right|}{\left| \frac{M(\alpha)}{\alpha h} (\chi_{0,h} - \bar{\chi}_{0,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right|} \\ &\leq 1. \end{aligned} \tag{8.1.13}$$

Clearly, assertion in (8.1.12) is true for  $k = 0$ . Let us also assume that it is true for the integer values  $2, 3, \dots, k$ , then using (8.1.11), we obtain

$$\begin{aligned} \delta_{k+1} &\left\{ \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right\} \\ &= \delta_k \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h^2} \sin^2 \left( \frac{\zeta_i}{2} \right) + \frac{2}{h^2} \right] \\ &\quad - \frac{M(\alpha)}{\alpha h} \left[ 2 \sum_{\substack{i=1 \\ i \neq k}}^{k+1} \delta_i \chi_{i,h} - 2 \sum_{i=1}^{k-1} \delta_i \bar{\chi}_{i,h} \right]. \end{aligned} \tag{8.1.14}$$

Further rearrangement gives

$$\begin{aligned} \delta_{k+1} &\left\{ \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h} + 2\chi_{k+1,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right\} \\ &= \delta_k \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h^2} \sin^2 \left( \frac{\zeta_i}{2} \right) + \frac{2}{h^2} \right] \\ &\quad - \frac{2M(\alpha)}{\alpha h} \sum_{i=1}^{k-1} \delta_i (\chi_{i,h} - \bar{\chi}_{i,h}). \end{aligned} \tag{8.1.15}$$

Without loss of generality, if we put  $M(\alpha) = 1$  as suggested in [13], then, after rearranging and making use of the recurrence hypothesis together with the coefficients (3.6.15)–(3.6.15), we have

$$\begin{aligned}
 \delta_{k+1} & \left\{ \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h} + 2\chi_{k+1,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right\} \\
 & = \left| \delta_k \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{0,h} - \chi_{0,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h^2} \sin^2 \left( \frac{\zeta_i}{2} \right) + \frac{2}{h^2} \right] \right. \\
 & \quad \left. - \frac{2M(\alpha)}{\alpha h} \sum_{i=1}^{k-1} \delta_i (\chi_{i,h} - \bar{\chi}_{i,h}) \right| \\
 & \leq \left| \delta_0 \left[ \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{0,h} - \chi_{0,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h^2} \sin^2 \left( \frac{\zeta_i}{2} \right) + \frac{2}{h^2} \right] \right. \\
 & \quad \left. - \frac{2M(\alpha)}{\alpha h} \left( \frac{-\alpha h}{4h^2} + \chi_{k+1,h} \right) \right|. \tag{8.1.16}
 \end{aligned}$$

Finally, we have

$$\begin{aligned}
 |\delta_{k+1}| & = |\delta_0| \frac{\left| \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h^2} \sin^2 \left( \frac{\zeta_i}{2} \right) + \frac{2}{h^2} + \frac{2M(\alpha)}{\alpha h} \left( \frac{-\alpha h}{4h^2} + \chi_{k+1,h} \right) \right|}{\left| \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h} + 2\chi_{k+1,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right|} \\
 & \leq |\delta_0| \frac{\left| \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) - \frac{4}{h^2} \sin^2 \left( \frac{\zeta_i}{2} \right) + \frac{2M(\alpha)}{\alpha h} \chi_{k+1,h} \right|}{\left| \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h} + 2\chi_{k+1,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right|} \\
 & \leq \frac{\left| \frac{M(\alpha)}{\alpha h} (\bar{\chi}_{k,h} - \chi_{k,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) + \frac{2M(\alpha)}{\alpha h} \chi_{k+1,h} \right|}{\left| \frac{M(\alpha)}{\alpha h} (\chi_{k,h} - \bar{\chi}_{k,h} + 2\chi_{k+1,h}) + \sin^2 \left( \frac{\zeta_i}{2} \right) \right|} \\
 & \leq 1. \tag{8.1.17}
 \end{aligned}$$

Hence, the following proposition is proved.

**Proposition 8.1.1** *Assume that the coefficients  $\delta_k$  satisfy Eqs. (8.1.9) and (8.1.11) for all  $k \geq 0$ , then, the numerical scheme is stable for the diffusion equation (8.1.1).*

## 8.2 Space-Fractional Diffusion Equation with the Riemann–Liouville Derivative

A space-fractional diffusion equation can be derived by replacing Fick’s law for the flux  $V$  (which represents the rate at which mass is transported through a unit area against the concentration gradient) by its fractional derivative, see, for instance, [12, 46]

$$V = -D \Delta^\alpha u, \quad 0 < \alpha \leq 1, \tag{8.2.1}$$

where  $D$  is the diffusion or conductivity tensor, and  $\Delta^\alpha = \left( \frac{\partial^\alpha}{\partial x^\alpha}, \frac{\partial^\alpha}{\partial y^\alpha}, \frac{\partial^\alpha}{\partial z^\alpha} \right)^T$  is the Riemann–Liouville fractional gradient, where

$$\frac{\partial^\alpha}{\partial x^\alpha} u(x, y, z) = \frac{1}{\Gamma(1-\alpha)} \frac{\partial}{\partial x} \int_0^x \frac{u(\xi, y, z)}{(x-\xi)} d\xi, \quad (8.2.2)$$

with similar expressions for  $\frac{\partial^\alpha}{\partial y^\alpha}$  and  $\frac{\partial^\alpha}{\partial z^\alpha}$  [12, 59, 64]. The fractional Fick's law (8.2.1) naturally means spatial and temporal non-locality, and can be derived from rigorous approaches via spatial averaging theorems and measurable functions. On adding this to a conservation of mass equation for the concentration of particles or species densities  $u(x, t)$

$$\partial_t u = -\Delta \cdot V, \quad (8.2.3)$$

which results in

$$\partial_t u = -D(-\Delta)^{\alpha/2} + f(u, t), \quad 1 < \alpha \leq 2, \quad (8.2.4)$$

where  $(-\Delta)^{\alpha/2}$  is simply the fractional Laplacian operator.

A classical way of solving problems of the form (8.2.4) is by applying a finite difference, finite element or finite volume discretization of the fractional operator [59], and then use a semi-implicit Euler formulation or any other time-stepping method for the time evolution of the solution.

A lot of numerical approaches have been used in the literature to overcome the non-local restrictions of space-fractional operators. A quick tour of such methods is presented as follows.

### 8.2.1 Fourier Transform Methods

Here, we familiarize with the definitions of the continuous and discrete fractional Fourier transforms.

**Definition 8.2.1** For a function  $u \in S(\mathbb{R})$  (Schwartzian space),  $S(\mathbb{R})$  being the space of rapidly decreasing test functions on the real axis  $\mathbb{R}$ , the Fourier transform  $\hat{u}$  is defined as

$$\hat{u}(\omega) = (\mathcal{F}u)(\omega) = \int_{-\infty}^{\infty} u(t)e^{i\omega t} dt, \quad \omega \in \mathbb{R}. \quad (8.2.5)$$

The inverse Fourier transform is given in the form

$$u(t) = (\mathcal{F}^{-1}\hat{u})(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{u}(\omega)e^{-i\omega t} d\omega, \quad t \in \mathbb{R}. \quad (8.2.6)$$

There are several definitions of the fractional Fourier transform in literature [12, 28, 38, 67]. Rather, we chose to stick to the ones that are of primary interests in the modelling of mathematical problems. Another focus in this work is to introduce our broad readers to some of the useful definitions of the fractional Fourier transform that are applicable to the solution of fractional differential problems.

**Definition 8.2.2** Let  $V(\mathbb{R})$  be the set of functions such that

$$V(\mathbb{R}) = \left\{ v \in S(\mathbb{R}) : \frac{d^n v}{d\wp^n} \Big|_{\wp=0} = 0, \quad n = 0, 1, 2, \dots \right\}. \quad (8.2.7)$$

The Lizorkin space  $\Phi(\mathbb{R})$  is defined as the Fourier preimage of the space  $V(\mathbb{R})$  in the space  $S(\mathbb{R})$ , i.e.

$$\Phi(\mathbb{R}) = \{\varphi \in S(\mathbb{R}) : \hat{\varphi} \in V(\mathbb{R})\}. \quad (8.2.8)$$

In other words, a function  $\varphi \in \Phi(\mathbb{R})$  if the orthogonality condition

$$\int_{-\infty}^{+\infty} \wp^n \varphi(\wp) d\wp = 0, \quad n = 0, 1, 2, \dots \quad (8.2.9)$$

is satisfied.

This operator was shown to remain invariant with respect to fractional integration and differentiation. This feature gives credit to the Lizorkin space to be a useful and versatile working tool with Fourier transform, fractional integration and differentiation operators. For further identities and details of the Lizorkin space, readers are referred to the classical book and research paper in [72, 73] and the references therein.

**Definition 8.2.3** For a function  $u \in \Phi(\mathbb{R})$ , the fractional Fourier transform of the order  $\alpha > 0$ ,  $\hat{u}_\alpha$ , is defined as

$$\hat{u}_\alpha(\omega) = (\mathcal{F}_\alpha u)(\omega) = \int_{-\infty}^{+\infty} e^{i \operatorname{sign}(\omega)|\omega|^{\frac{1}{\alpha}} t} u(t) dt, \quad \omega \in \mathbb{R}, \quad (8.2.10)$$

and the inverse fractional Fourier transform of order  $\alpha > 0$  is given by

$$(\mathcal{F}_\alpha^{-1} u)(\omega) = \frac{1}{2\pi\alpha} \int_{-\infty}^{+\infty} e^{-i \operatorname{sign}(\omega)|\omega|^{\frac{1}{\alpha}} t} \hat{u}_\alpha(\omega) \omega^{\frac{1-\alpha}{\alpha}} d\omega, \quad t \in \mathbb{R}. \quad (8.2.11)$$

Hence, we have

$$\mathcal{F}_\alpha^{-1} \mathcal{F}_\alpha u = u. \quad (8.2.12)$$

One can see clearly that for  $\alpha = 1$ , the fractional Fourier transform  $\mathcal{F}_\alpha$  is reduced to the conventional Fourier transform  $\mathcal{F}$ . These transforms are connected by the relation

$$\hat{u}_\alpha(\omega) = (\mathcal{F}_\alpha u)(\omega) = (\mathcal{F}u)(\wp) = \hat{u}(\wp), \quad \wp = \operatorname{sign}(\omega)|\omega|^{\frac{1}{\alpha}}. \quad (8.2.13)$$

The properties of fractional Fourier transform on derivatives are given in the following theorems.

**Theorem 8.2.4** *Let  $u$  be a function which belongs to the Lizorkins space  $\Phi(\mathbb{R})$ , and  $\wp \in \mathbb{R}$*

$$\mathcal{F}_\alpha \left( \frac{d^n}{dt^n} u(t) \right) (\omega) = (-i \operatorname{sign}(\omega) |\omega|^{\frac{1}{\alpha}})^n (\mathcal{F}_\alpha u)(\omega). \tag{8.2.14}$$

*In particular,*

$$\mathcal{F} \left( \frac{d^n}{dt^n} u(t) \right) (\omega) = (-i\omega)^n (\mathcal{F}u)(\omega). \tag{8.2.15}$$

The proof of Theorem 8.2.4 follows from relation (8.2.13).

**Theorem 8.2.5** ([29]) *Let  $\alpha > 0$ ,  $\beta \in \mathbb{R}$  and let a function  $u$  belong to the Lizorkin space  $\Phi(\mathbb{R})$ . The following operational relation is satisfied for all values of  $\beta$ :*

$$(\mathcal{F}_\alpha D_\beta^\alpha u)(\omega) = (-i c_\alpha(\beta)\omega)(\mathcal{F}_\alpha u)(\omega), \quad (\alpha > 0; \beta, \omega \in \mathbb{R}), \tag{8.2.16}$$

where  $c_\alpha$  is a constant defined as

$$c_\alpha = \sin(\alpha\pi/2) + i \operatorname{sign}(\omega)(1 - 2\beta) \cos(\alpha\pi/2). \tag{8.2.17}$$

*In particular, in the case  $\beta = \frac{1}{2}$ , we have*

$$(\mathcal{F}_\alpha D_{1/2}^\alpha u)(\omega) = -i \sin(\alpha\pi/2)\omega(\mathcal{F}_\alpha u)(\omega), \quad (\alpha > 0; \beta, \omega \in \mathbb{R}) \tag{8.2.18}$$

*for the fractional derivative*

$$D_{1/2}^\alpha u = \frac{1}{2}(D_+^\alpha u - D_-^\alpha u), \quad \alpha > 0. \tag{8.2.19}$$

The proof of Theorem 8.2.5 is omitted here, see [30] for details.

### 8.2.2 Finite Difference Methods

Finite difference method of approximation is not new in the literature, they are typically defined on well-structured grids. In the case of the fractional operator, two approaches may be taken. The first is to apply the fractional power to the finite difference Laplacian matrix. That is, take the matrix representation, say  $\mathbf{L}$ , of the Laplacian and raise it to the desired fractional power of order  $\alpha$ . Second, a finite difference formula on tensor grids using a shifted Grunwald [45, 69] approximation can be applied. When discretized in two- and three-dimensional space, this approach provides a well-structured, relatively sparse and positive definite matrices. The solution of both linear and nonlinear systems can be approximated effectively also by the combination of conjugate gradient and multi-grid methods. As well as relying on

having simple geometries, finite difference approximations have its own shortcomings because they are not capable of exploiting solutions with high regularity.

For the approximation of above equation using finite difference, we discretized the spatial domain  $[l_1, l_2]$   $N$  uniformly into subintervals of size  $\Delta\wp = (l_2 - l_1)/N$ . In a similar manner, we discretize the time domain  $0 \leq t \leq T$  with  $M$  subintervals of size  $\Delta t = T/M$ . The spatial and time grid points are denoted, respectively, as  $\wp_i = l_1 + i\Delta\wp$ ,  $i = 0, 1, 2, \dots, N$  and  $t_j = j\Delta t$ ,  $j = 0, 1, 2, \dots, M$ .

For us to apply the second-order approximations of the spatial fractional derivative and a second-order approximation for the time derivative, the space-fractional-order reaction–diffusion equation is written in a shifted form for both spatial and time variables as

$$D_t u(\wp + \varphi\Delta\wp, t + \Delta t/2) = \delta(\wp + \varphi\Delta\wp) D_\wp^\alpha u(\wp + \varphi\Delta\wp, t + \Delta t/2) + \mathcal{F}(\wp + \varphi\Delta\wp, t + \Delta t/2), \tag{8.2.20}$$

where  $D_t u = \partial/\partial t$  and  $D_\wp^\alpha = \partial^\alpha/\partial\wp^\alpha$ . For detailed derivation and analysis, readers are referred to the literature.

### 8.2.3 Predictor–Corrector Method of Approximation

Let us consider the following space-fractional-order reaction–diffusion equation

$$\partial_t u = \delta \Delta^\alpha u + \mathcal{F}(u, t), \quad l_1 < \wp < l_2, \quad 0 < t \leq T \tag{8.2.21}$$

subject to initial and boundary conditions

$$\begin{aligned} u(\wp, 0) &= u_0(\wp), \quad l_1 < \wp < l_2 \\ u(l_1, t) &= 0, \quad 0 < t \leq T \\ u(l_2, t) &= 0, \quad 0 < t \leq T, \end{aligned} \tag{8.2.22}$$

where  $\Delta^\alpha u = \frac{\partial^\alpha u(\wp, t)}{\partial|\wp|^\alpha}$ ,  $\delta$  remains the diffusion tensor or conductivity and  $\mathcal{F}$  as earlier defined. In the spirits of [56, 61], we discretize Eqs. (8.2.21) and (8.2.22) to obtain

$$\hat{u}_i^{j+1} = u_i^j - \frac{\delta\eta}{h^\alpha} \sum_{k=-m+i}^i g_k u_i^j - k + \eta \mathcal{F}_i^{j+\frac{1}{2}} \tag{8.2.23}$$

as the *predictor*, and

$$u_i^{j+1} = \frac{1}{2} \left( u_i^j + \hat{u}_i^{j+1} - \delta\eta h^{-\alpha} \sum_{k=-m+i}^i g_k \hat{u}_i^{j+1} - k + \eta \mathcal{F}_i^{j+\frac{1}{2}} \right) \tag{8.2.24}$$

as the corrector. For  $i = 1, 2, \dots, m - 1$  and  $j = 0, 1, \dots, N - 1, h = \frac{l_2 - l_1}{m}, \eta = \frac{T}{N}, t_j = j\eta, \wp_i = l_1 + ih$  and  $u_i^j = u(\wp_i, t_j)$ .

Using vector-matrix notation, we can present Eqs.(8.2.23) and (8.2.24) in the form

$$U^{j+1} = \frac{1}{2} \left( U^j + (\mathbf{I} - \mathbf{L}_1)\hat{U}^{j+1} + \eta \mathbf{F}^{j+\frac{1}{2}} \right), \tag{8.2.25}$$

$$\hat{U}^{j+1} = (\mathbf{I} - \mathbf{L}_1)U^j + \mathbf{L}_2 + \eta \mathbf{F}^{j+\frac{1}{2}},$$

where

$$U^j = (u_1^j, u_2^j, \dots, u_{m-1}^j)^T \text{ and } \mathbf{F}^{j+\frac{1}{2}} = \left( \mathcal{F}_1^{j+\frac{1}{2}}, \mathcal{F}_2^{j+\frac{1}{2}}, \dots, \mathcal{F}_{m-1}^{j+\frac{1}{2}} \right)^T.$$

In this case,  $\mathcal{F}_i^{j+\frac{1}{2}} = \mathcal{F}(\wp_i, t_{j+\frac{1}{2}}), t_{j+\frac{1}{2}} = j\eta + \eta/2, \mathbf{L}_1$  is defined as a matrix of size  $(m - 1) \times (m - 1), l_1 = \eta\delta/h^\alpha$  with elements  $\rho_k = \rho_{-k}$  and  $\mathbf{L}_2$  is a column vector with given boundary conditions.

$$\mathbf{L}_1 = \begin{pmatrix} l_1\rho_0 & l_1\rho_{-1} & l_1\rho_{-2} & \cdots & l_1\rho_{-m+2} \\ l_1\rho_1 & l_1\rho_0 & l_1\rho_{-1} & \cdots & l_1\rho_{-m+3} \\ l_1\rho_2 & l_1\rho_1 & l_1\rho_0 & \cdots & l_1\rho_{-m+4} \\ \vdots & \vdots & \vdots & \ddots & \\ l_1\rho_{m-2} & l_1\rho_{m-3} & l_1\rho_{m-4} & \cdots & l_1\rho_0 \end{pmatrix}, \mathbf{L}_2 = \begin{pmatrix} \rho_1 u_0 + \rho_{-m+1} u_m \\ \rho_2 u_0 + \rho_{-m+2} u_m \\ \rho_3 u_0 + \rho_{-m+3} u_m \\ \vdots \\ \rho_{m-1} u_0 + \rho_{-m+1} u_m \end{pmatrix}. \tag{8.2.26}$$

### Stability Analysis of the Predictor–Corrector Method

We use the following theorem result to show that the proposed method is stable.

**Theorem 8.2.6** *The discretized Eq.(8.2.25) is conditionally stable for the space-fractional-order reaction–diffusion equations (8.2.21) and (8.2.22).*

*Proof* Assume  $\lambda$  to be the eigenvalue of the matrix  $\mathbf{L}_1$ . By adopting the Gershgorin circle theorem [54], we obtain

$$|\lambda - l_1\rho_0| \leq \tau_i = l_1 \sum_{k=-m+i}^{i-1} |\rho_k| < l_1\rho_0.$$

Known that  $\sum_{k=-\infty}^{\infty} |\rho_k| = \rho_0$ , hence

$$0 < \lambda < 2l_1\rho_0.$$

Combination of the predictor–corrector method

$$U^{j+1} = \frac{1}{2} \left( U^j + (\mathbf{I} - \mathbf{L}_1)\hat{U}^{j+1} + \eta\mathbf{F}^{j+\frac{1}{2}} \right),$$

$$\hat{U}^{j+1} = (\mathbf{I} - \mathbf{L}_1)U^j + \mathbf{L}_2 + \eta\mathbf{F}^{j+\frac{1}{2}},$$

yields

$$u^{j+1} = \frac{1}{2} \left\{ U^j + (\mathbf{I} - \mathbf{L}_1) \left[ (\mathbf{I} - \mathbf{L}_1)U^j + \mathbf{L}_2 + \eta\mathbf{F}^{j+\frac{1}{2}} \right] \eta\mathbf{F}^{j+\frac{1}{2}} \right\}. \quad (8.2.27)$$

For stability to be attained, the eigenvalue  $\frac{|\mathbf{I} + (\mathbf{I} - \mathbf{L}_2)^2|}{2}$  must satisfy the condition

$$\frac{|1 + 2(1 - \lambda)(1 - \lambda)|}{2} < 1. \quad (8.2.28)$$

Hence,  $2l_1\rho_0 < 2$  and  $l_1 = \frac{\eta}{h^\alpha} < \frac{1}{\rho_0}$ , and therefore Eq. (8.2.22) is conditionally stable.  $\square$

**Definition 8.2.7** The inequality in (8.2.28) gives a sufficient condition for the stability of the predictor–corrector scheme (8.2.27) for the space-fractional-order reaction–diffusion equation and is called the CFL (Courant–Friedrichs–Lewy) condition.

### 8.2.4 Fourier Spectral Method for Space-Fractional Reaction–Diffusion

Spectral methods are approximation techniques for the computation of the solutions to ordinary and partial differential equations. They are based on a polynomial expansion of the solution. The precision of these methods is limited only by the regularity of the solution, in contrast to the finite difference and finite element methods. Knowing well that the nature of problem allows the use of two classical methods, one in space and the other in time. As a result, we intend using Fourier spectral method to discretize in space, and then advance the resulting system of ordinary differential equations with the modified version of the exponential time-differencing schemes

[15, 27]. To present this approach, we first write the fractional reaction–diffusion equation in the general form

$$\left. \begin{aligned} \frac{\partial u(\wp, t)}{\partial t} &= \delta(\Delta)^\alpha u(\wp, t) + \mathcal{F}(u, t), \quad 0 < \alpha \leq 2, \\ u(\wp, 0) &= u_0(\wp), \end{aligned} \right\} \quad (8.2.29)$$

where  $u = (\mathcal{U}, \cdot)^T \in \mathbb{R}^n$  are the species densities in one  $\wp = (x)$ , two  $\wp = (x, y)^T$  or three  $\wp = (x, y, z)^T$  dimensions,  $\delta = (\delta_i), i = 1, 2, 3 \in \mathbb{R}_+$  are their constant matrices which describe the respective diffusion coefficients. The operator  $(\Delta)^\alpha$  remains the fractional Laplacian operator associated with the species, and the term  $\mathcal{F}(u, t)$  represents the biological or chemical reactions.

Though there are several existing numerical methods that can be used to discretize (8.2.29) in space. It should be noted that the fractional differential operator is non-local red operator, which often results in a serious computational and numerical challenges that are rarely encountered in the context of classical second-order reaction–diffusion equations. In addition, for the space-fractional diffusion equations, most numerical techniques often result in full coefficient matrices with complicated structures [44]. In this chapter, we employ fractional Fourier spectral methods [30] to discretize the space-fractional derivatives.

Next, we apply the fractional Fourier transform operator  $F_\alpha$  (8.2.10) on both sides of (8.2.29), making use formula (8.2.16), to obtain the ODEs system

$$\left. \begin{aligned} \frac{\partial \hat{u}_\alpha}{\partial t}(\omega, t) &= \delta(i c_\alpha(\beta)\omega) \hat{u}_\alpha(\omega, t) + \widehat{\mathcal{F}_\alpha(u, t)}, \quad 0 < \alpha \leq 2, \\ \hat{u}_\alpha(\omega, 0) &= \hat{u}_{\alpha,0}(\omega), \end{aligned} \right\} \quad (8.2.30)$$

where  $c_\alpha$  is a constant defined as

$$c_\alpha = \sin(\alpha\pi/2) + i \text{sign}(\omega)(1 - 2\beta) \cos(\alpha\pi/2). \quad (8.2.31)$$

This approach yields a full diagonal representation of the fractional operator and provides a better spectral convergence irregardless of the fractional power in the given problem.

By relaxing the condition imposed on fractional power to unity, and by using Eqs. (8.2.5) and (8.2.6) we can write the 2D Fourier transform of a function  $u(x, y)$  as

$$\mathcal{F}(u)(k_x, k_y) = \hat{u}(k_x, k_y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i(k_x x + k_y y)} u(x, y) dx dy$$

with the corresponding inverse Fourier transform

$$\mathcal{F}^{-1}(\hat{u})(x, y) = u(x, y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i(k_x x + k_y y)} \hat{u}(k_x, k_y) dk_x dk_y.$$

One can interpret the function  $\hat{u}(k_x, k_y)$  as the amplitude density of  $u$  for the wave numbers  $k_x$  and  $k_y$ . Application to higher spatial dimensions is practically the same as illustrated to one- and two-dimensional problems above. Careful attention should be given in order to filter the occurrence of high frequencies appropriately, since the nonlinear term is evaluated in physical space and then transformed to Fourier space. This can lead to problems with aliasing [27, 63].

The essential point is that once the stiffness issue is removed one can employ any explicit higher order time integrators to rapidly and accurately advance forwards in time, and this is vastly superior to the use of implicit schemes most especially in higher dimensions. Hence, for the temporal discretization, we engage an improved fourth-order exponential time-differencing Runge–Kutta (ETDRK4) scheme as proposed by Cox and Matthews [15], which was later modified by Kassam and Trefethen [27] as

$$\begin{aligned}
 a_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1} (e^{\mathbf{L}h/2} - \mathbf{I}) \mathbf{F}(u_n, t_n), \\
 b_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1} (e^{\mathbf{L}h/2} - \mathbf{I}) \mathbf{F}(a_n, t_n + h/2), \\
 c_n &= e^{\mathbf{L}h/2}u_n + \mathbf{L}^{-1} (e^{\mathbf{L}h/2} - \mathbf{I}) [2\mathbf{F}(b_n, t_n + h/2) - \mathbf{F}(u_n, t_n)], \\
 u_{n+1} &= e^{\mathbf{L}h}u_n + h^{-2}\mathbf{L}^{-3}\{[-4\mathbf{I} - h\mathbf{L} + e^{\mathbf{L}h}(4\mathbf{I} - 3h\mathbf{L} + (h\mathbf{L})^2)]\mathbf{F}(u_n, t_n) \\
 &\quad + 2[2\mathbf{I} + h\mathbf{L} + e^{\mathbf{L}h}(-2\mathbf{I} + h\mathbf{L})](\mathbf{F}(a_n, t_n + h/2) + \mathbf{F}(b_n, t_n + h/2)) \\
 &\quad + [-4\mathbf{I} - 3h\mathbf{L} - (h\mathbf{L})^2 + e^{\mathbf{L}h}(4\mathbf{I} - h\mathbf{L})]\mathbf{F}(c_n, t_n + h)\}. \tag{8.2.32}
 \end{aligned}$$

To save time and avoid repetition, information on derivation, stability and convergence of the ETDRK4 and other explicit exponential integrators can be found in [15, 27, 57, 61, 63].

### 8.3 Application of Caputo–Fabrizio Derivative to Nonlinear Reaction–Diffusion

The fractional derivatives are known to be remembrance operative with which we often characterize dissoluteness of energy or smash up in the middling as in the case of inelastic media or re-evaluation of the porosity in the leaky media, additionally in a wide range being in conformity with the previous theory of thermodynamics. Model representation with fractional derivative operators has been shown to be more accurate and reliable when compared to the integer-order cases [30, 69]. Here, we present the analysis of nonlinear Fisher reaction–diffusion equation with time-fractional Caputo–Fabrizio derivative. Equation for consideration is given as

$${}_0^CF_t^\alpha u(x, t) = \gamma \frac{\partial^2 u(x, t)}{\partial x^2} - \beta u(x, t)(1 - u^p(x, t)), \quad p > 1, \quad 0 < \gamma < 1 \tag{8.3.1}$$

subject to the initial condition

$$u(x, 0) = 0, \quad a \leq x \leq b. \tag{8.3.2}$$

### 8.3.1 Derivation of the Solution via Iterative Method

In this section, we derive the solution of (8.3.1) via an iterative technique. By applying the Sumudu transform [4] on both sides of (8.3.1), we have

$$M(\alpha) \frac{sSF(u(x, t)) - u(x, 0)}{1 - \alpha + \alpha s} = SL \left\{ \gamma \frac{\partial^2 u(x, t)}{\partial x^2} - \beta u(x, t)(1 - u^p(x, t)) \right\}. \tag{8.3.3}$$

On rearranging gives

$$SF(u(x, t)) = \frac{u(x, 0)}{s} + \frac{1 + (\alpha - 1)s}{sM(\alpha)} SL \left\{ \gamma \frac{\partial^2 u(x, t)}{\partial x^2} - \beta u(x, t)(1 - u^p(x, t)) \right\}. \tag{8.3.4}$$

Next, we apply the inverse Sumudu transform on both sides of (8.3.4), to have

$$u(x, t) = u(x, 0) + SL^{-1} \left\{ \frac{1 + (\alpha - 1)s}{sM(\alpha)} SL \left\{ \gamma \frac{\partial^2 u(x, t)}{\partial x^2} - \beta u(x, t)(1 - u^p(x, t)) \right\} \right\}.$$

We next obtain the recursive formula

$$u(x, 0) = u_o(x, t)$$

$$u_{n+1}(x, t) = u_n(x, t) + SL^{-1} \left\{ \frac{1 + (\alpha - 1)s}{sM(\alpha)} SL \left( \gamma \frac{\partial^2 u_n(x, t)}{\partial x^2} - \beta u_n(x, t)(1 - u_n^p(x, t)) \right) \right\}. \tag{8.3.5}$$

The solution of the time-fractional Fisher equation (8.3.1) is given as

$$u(x, t) = \lim_{n \rightarrow \infty} u_n(x, t). \tag{8.3.6}$$

### 8.3.2 Stability Analysis via Fixed Point Theorem

Suppose  $(X, \| \cdot \|)$  is a Banach space, and  $A$  a self-map of  $X$ . Let  $z_{n+1} = g(A, z_n)$  be particular recursive process. Suppose that,  $G(A)$  the fixed point set of  $A$  has at least one element and that  $z_n$  converges to a point  $s \in G(A)$ . Let  $\{x_n\} \subseteq X$  and define  $e^n = \|x_{n+1} - g(A, x_n)\|$ . If  $\lim_{n \rightarrow \infty} e^n = 0$  means that  $\lim_{n \rightarrow \infty} x^n = s$ , then the iteration method  $z_{n+1} = g(A, z_n)$  is said to be  $A$ -stable. Without loss of generality, we suppose that our sequence  $x_n$  has an upper boundary, otherwise convergence will be impossible.

If all these conditions are satisfied for  $z_{n+1} = Az_n$  which is referred to as Picard’s iteration, consequently the iteration is  $A$ –stable. Now, we proceed with the following theorem.

**Theorem 8.3.1** (Odibat and Momani [52]) *Suppose  $(X, \|\cdot\|)$  is a Banach space, and  $A$  a self-map of  $X$  satisfying*

$$\|A_x - A_z\| \leq C\|x - A_x\| + c\|x - z\|$$

for all  $x, z \in X$  where  $0 \leq C, 0 \leq c < 1$ . Suppose that  $A$  is Picard  $A$ –stable.

Let us consider the following succession which correlates to the nonlinear fractional Fisher’s equation:

$$u_{n+1}(x, t) = u_n(x, t) + SL^{-1} \left\{ \frac{1 + (\alpha - 1)s}{sM(\alpha)} SL \left\{ \begin{array}{c} \gamma \frac{\partial^2 u_n(x, t)}{\partial x^2} \\ -\beta u_n(x, t)(1 - \bar{u}_n^p(x, t)) \end{array} \right\} \right\},$$

where  $\frac{1+(\alpha-1)s}{sM(\alpha)}$  stands for the fractional Lagrange multiplier and  $\bar{u}_n^p$  is a restricted variation indicating that  $\delta \bar{u}_n^p = 0$ .

**Theorem 8.3.2** *Let  $S$  be a self-map defined as*

$$\begin{aligned} S(u_n(x, t)) &= u_{n+1}(x, t) \\ &= u_n(x, t) + SL^{-1} \left\{ \frac{1 + (\alpha - 1)s}{sM(\alpha)} SL \left\{ \begin{array}{c} \gamma \frac{\partial^2 u_n(x, t)}{\partial x^2} \\ -\beta u_n(x, t)(1 - \bar{u}_n^p(x, t)) \end{array} \right\} \right\} \end{aligned}$$

is  $S$ –stable in  $L^2(a, b)$  if

$$\left\{ \frac{\gamma\beta_1\beta_2 + (C + B)^p\beta}{M(\alpha)}\alpha + \frac{\alpha}{M(\alpha)} \right\} < \beta.$$

*Proof* We first show that  $S$  has a fixed point. To arrive at this, we evaluate the following for all  $(n, k) \in N \times N$ :

$$\begin{aligned} &\|S(u_n(x, t)) - S(u_k(x, t))\| \\ &= \left\| \begin{array}{c} u_n(x, t) - u_k(x, t) \\ +SL^{-1} \left\{ \frac{1+(\alpha-1)s}{sM(\alpha)} SL \left\{ \begin{array}{c} \gamma \frac{\partial^2 u_n(x, t)}{\partial x^2} \\ -\beta u_n(x, t)(1 - \bar{u}_n^p(x, t)) \end{array} \right\} \right\} \\ -SL^{-1} \left\{ \frac{1+(\alpha-1)s}{sM(\alpha)} SL \left\{ \begin{array}{c} \gamma \frac{\partial^2 u_k(x, t)}{\partial x^2} \\ -\beta u_k(x, t)(1 - \bar{u}_k^p(x, t)) \end{array} \right\} \right\} \end{array} \right\|. \end{aligned}$$

Using the linearity property of the inverse Sumudu transform, we have

$$\begin{aligned} & \|S(u_n(x, t)) - S(u_k(x, t))\| \\ &= \left\| \begin{aligned} & u_n(x, t) - u_k(x, t) \\ & +SL^{-1} \left\{ \frac{1+(\alpha-1)s}{sM(\alpha)} SL \left\{ \begin{aligned} & \gamma \frac{\partial^2 \{u_n(x,t) - u_k(x,t)\}}{\partial x^2} \\ & -\beta \{u_n(x, t) - u_k(x, t)\} \end{aligned} \right\} \right\} \\ & +\beta \left\{ u_n^{p+1}(x, t) - u_k^{p+1}(x, t) \right\} \end{aligned} \right\|. \end{aligned}$$

In addition, by using the triangular inequality for the norm, we obtain

$$\begin{aligned} & \|S(u_n(x, t)) - S(u_k(x, t))\| \\ & \leq \|u_n(x, t) - u_k(x, t)\| + \left\| \begin{aligned} & u_n(x, t) - u_k(x, t) \\ & +SL^{-1} \left\{ \frac{1+(\alpha-1)s}{sM(\alpha)} SL \left\{ \begin{aligned} & \gamma \frac{\partial^2 \{u_n(x,t) - u_k(x,t)\}}{\partial x^2} \\ & -\beta \{u_n(x, t) - u_k(x, t)\} \end{aligned} \right\} \right\} \\ & +\beta \left\{ u_n^{p+1}(x, t) - u_k^{p+1}(x, t) \right\} \end{aligned} \right\|. \end{aligned} \tag{8.3.7}$$

With property of norm and integral, the above is transformed as follows:

$$\begin{aligned} & \|S(u_n(x, t)) - S(u_k(x, t))\| \leq \|u_n(x, t) - u_k(x, t)\| \\ & +SL^{-1} \left\{ \frac{1+(\alpha-1)s}{sM(\alpha)} SL \left\{ \left\| \gamma \frac{\partial^2 \{u_n(x, t) - u_k(x, t)\}}{\partial x^2} \right\| \right\} \right\} \\ & +SL^{-1} \left\{ \frac{1+(\alpha-1)s}{sM(\alpha)} SL \left\{ \left\| -\beta \{u_n(x, t) - u_k(x, t)\} \right\| \right\} \right\} \\ & +SL^{-1} \left\{ \frac{1+(\alpha-1)s}{sM(\alpha)} SL \left\{ \left\| -\beta \{u_n^{p+1}(x, t) - u_k^{p+1}(x, t)\} \right\| \right\} \right\}. \end{aligned} \tag{8.3.8}$$

Evaluation of Eq. (8.3.8) can be treated case by case, beginning with

$$\left\| \gamma \frac{\partial^2 \{u_n(x, t) - u_k(x, t)\}}{\partial x^2} \right\| \leq \gamma \beta_1 \beta_2 \|u_n(x, t) - u_k(x, t)\|.$$

Followed by

$$\begin{aligned} & \|\beta \{u_n^{p+1}(x, t) - u_k^{p+1}(x, t)\}\| \\ & \leq \left\| \sum_{j=0}^p C_m^j (u_n(x, t))^j (u_k(x, t))^{p-j-1} \right\| \|u_n(x, t) - u_k(x, t)\|. \end{aligned} \quad (8.3.9)$$

Since both  $u_n(x, t)$  and  $u_k(x, t)$  are bounded, we can find two different positive constants,  $C$  and  $B$ , such that for all  $x, t$ ,

$$\|u_n(x, t)\| < C, \quad \|u_k(x, t)\| < B, \quad (n, k) \in \mathbb{N} \times \mathbb{N}.$$

Therefore, using the triangular inequality with the inequality in (8.3.9) gives

$$\|\beta \{u_n^{p+1}(x, t) - u_k^{p+1}(x, t)\}\| \leq (C + B)^p \|u_n(x, t) - u_k(x, t)\|. \quad (8.3.10)$$

By putting Eqs. (8.3.9) and (8.3.10) into (8.3.8), one obtains

$$\begin{aligned} & \|S(u_n(x, t)) - S(u_k(x, t))\| \\ & \leq \left\{ 1 - \beta + \frac{\gamma\beta_1\beta_2 + (C + B)^p\beta}{M(\alpha)}\alpha + \frac{\alpha}{M(\alpha)} \right\} \|u_n(x, t) - u_k(x, t)\| \end{aligned} \quad (8.3.11)$$

with

$$\left\{ \frac{\gamma\beta_1\beta_2 + (C + B)^p\beta}{M(\alpha)}\alpha + \frac{\alpha}{M(\alpha)} \right\} < \beta.$$

Then, the nonlinear  $S$ –self-mapping has a fixed point. The proof is completed. Next, we show that  $S$  also holds for the conditions in Theorem 8.3.1. Suppose the following Laplace transform

$$\mathcal{L}({}_0^{CF}\mathcal{D}_t^\alpha(f(t))) (q) = \frac{M(\alpha)}{1 - \alpha} \mathcal{L}\left(\frac{df(x)}{dx}\right) \mathcal{L}\left(\exp\left(-\alpha \frac{t}{1 - \alpha}\right)\right) \quad (8.3.12)$$

holds, thus putting

$$d = 0, \quad D = \left\{ 1 - \beta + \frac{\gamma\beta_1\beta_2 + (C + B)^p\beta}{M(\alpha)}\alpha + \frac{\alpha}{M(\alpha)} \right\}$$

implies that conditions of Theorem 8.3.1 satisfy for the nonlinear mapping  $S$ . Therefore, since all conditions in Theorem 8.3.1 are satisfied for the given nonlinear mapping  $S$ , then  $S$  is said to be Picard's  $S$ –stable. Hence, the proof of Theorem 8.3.2 is completed.  $\square$

### 8.4 Application of Caputo–Fabrizio Derivative to Transmission Line Model with Losses

The model under investigation is given as [71]

$$\frac{\partial^2 U(x, t)}{\partial x^2} - \frac{LC \partial^2 U(x, t)}{\partial t^2} - (RC + GL) \frac{\partial U(x, t)}{\partial t} - GRU(x, t) = 0, \quad (8.4.1)$$

where  $L$  is the representation of the inductance due to the presence of the magnetic field around the wires,  $C$  stands for the capacitance between the two conductors,  $R$  is the resistance of the conductors and  $G$  is the conductance of the electric material separating the conductors. Using the proposed transition, Atangana and Nieto [8] suggested the following fractional  $RLC$  circuit model:

$$\begin{aligned} & \frac{1}{\exp\left[-\frac{\beta\sigma_x}{2-\beta}\right]} {}_0^{CF} \mathcal{D}_x^\beta(U(x, t)) - \frac{LC}{\exp\left[-\frac{\beta\sigma_t}{2-\beta}\right]} {}_0^{CF} \mathcal{D}_t^\beta(U(x, t)) \\ & - \frac{(RC + GL)}{\exp\left[-\frac{(1-\alpha)\sigma_t}{2-\beta}\right]} \left\{ {}_0^{CF} \mathcal{D}_t^\alpha(U(x, t)) \right\} - GRU(x, t) = 0 \end{aligned} \quad (8.4.2)$$

with  $0 < \alpha < 1$  and  $1 < \beta < 2$ .

In what follows, we shall present the numerical solution of the time-fractional transmission line with losses using the Caputo–Fabrizio fractional derivative.

Given some positive integer, say  $N$ , the grid sizes in time for finite difference approach is defined by

$$k = \frac{i}{N}.$$

The grid points in the time interval  $[0, T]$  are denoted as  $t_n = nk$ ,  $n = 0, 1, 2, \dots, TN$ . For some  $N > 0$ , the grid sizes in time for finite difference method are given by

$$i = \frac{1}{M}.$$

The grid points in the space interval  $[0, X]$  are represented as  $x_i = im$ ,  $m = 0, 1, 2, \dots, XM$ . We consider the modified model of transmission line with losses (8.4.2) subject to the initial and boundary conditions

$$U(x, 0) = f(x), \quad U(0, t) = g(t).$$

Our main objective here is to numerically solve the above equation with the aid of the Crank–Nicholson scheme. To achieve this objective, we first replace in Eq. (8.4.2) the numerical approximations of space- and time-fractional Caputo–Fabrizio derivative, and this gives

$$\begin{aligned}
 & \frac{1}{\exp\left[-\frac{\beta\sigma_x}{1-\beta}\right]} \left\{ \frac{1}{2} \sum_{i=1}^m \left\{ \frac{(U_{i+1}^{k+1} - 2U_i^{k+1} + U_{i-1}^{k+1}) + (U_{i+1}^k - 2U_i^k + U_{i-1}^k)}{2(\Delta x)^2} \right\} \right. \\
 & \quad \times \left. \left\{ \operatorname{erf}\left[\frac{\beta}{1-\beta}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\beta}{1-\beta}(x_j - x_k)\right] \right\} \right\} \\
 & - \frac{LC}{\exp\left[-\frac{\beta\sigma_t}{2-\beta}\right]} \left\{ \frac{1}{2} \sum_{k=1}^j \left\{ \frac{(U_{i+1}^{k+1} - 2U_i^{k+1} + U_{i-1}^{k+1})}{2(\Delta t)^2} \right\} \right. \\
 & \quad \times \left. \left\{ \operatorname{erf}\left[-\frac{\beta k}{1-\beta}(n-j+1)\right] - \operatorname{erf}\left[-\frac{\beta k}{1-\beta}(n-j)\right] \right\} \right\} \\
 & - \frac{(RC + GL)}{\exp\left[-\frac{(\alpha)\sigma_t}{1-\alpha}\right]} \left\{ \frac{M(\alpha)}{\alpha} \sum_{k=1}^j \left( \frac{U_i^{k+1} - U_i^k}{\Delta t} \right) \exp\left[-\alpha \frac{k}{1-\alpha}(n-j+1)\right] \right. \\
 & \quad \left. - \exp\left[\alpha \frac{k}{1-\alpha}(n-j)\right] \right\} - GR \left( \frac{U_i^{j+1} - U_i^j}{2} \right) = 0. \tag{8.4.3}
 \end{aligned}$$

For the sake of simplicity, we let

$$\begin{aligned}
 g_{n,j,k} &= \exp\left[-\alpha \frac{k}{1-\alpha}(n-j+1)\right] - \exp\left[-\alpha \frac{k}{1-\alpha}(n-j)\right], \\
 \mu_{n,j,k} &= \left\{ \operatorname{erf}\left[\frac{\alpha}{1-\alpha}(x_j - x_{k+1})\right] - \operatorname{erf}\left[\frac{\alpha}{1-\alpha}(x_j - x_k)\right] \right\}, \\
 p_\alpha &= \frac{(RC + GL)}{2(\Delta t) \exp\left[-\frac{(\alpha)\sigma_t}{1-\alpha}\right]} \frac{M(\alpha)}{\alpha}, \\
 u_\alpha &= \frac{LC}{2(\Delta t)^2 \exp\left[-\frac{\beta\sigma_t}{2-\beta}\right]}, \\
 \nu_\beta &= \frac{1}{2(\Delta x)^2 \exp\left[-\frac{\beta\sigma_x}{2-\beta}\right]}.
 \end{aligned}$$

### 8.4.1 Stability Analysis of the Numerical Scheme with the Caputo–Fabrizio Derivative

In this section, we will adapt the Fourier method to establish the stability condition of the numerical scheme used to solve the modified model of time-fractional transmission line with losses. Equation (8.4.3) now becomes

$$\begin{aligned}
& \nu_\beta \left\{ \frac{1}{2} \sum_{s=1}^i \left\{ \left( U_{s+1}^{j+1} - 2U_s^{j+1} + U_{s-1}^{j+1} \right) + \left( U_{s+1}^j - 2U_s^j + U_{s-1}^j \right) \right\} \mu_{i,j,s} \right\} \\
& - u_\alpha \left\{ \frac{1}{2} \sum_{k=1}^j \left\{ U_{i+1}^{k+1} - 2U_i^{k+1} + U_{i-1}^{k+1} \right\} \mu_{n,j,k} \right\} - p_\alpha \left\{ \sum_{k=1}^j \left( U_i^{k+1} - U_i^k \right) g_{n,j,k} \right\} \\
& - GR \left( \frac{U_i^{j+1} - U_i^j}{2} \right) = 0. \tag{8.4.4}
\end{aligned}$$

We put  $\beta_i^j = u_i^j - U_i^j$  with  $U_i^j$  representing the approximate solution at the collocation point  $(x_i, t_j)$  and the vector  $\beta^j = [\beta_1^j, \beta_2^j, \dots, \beta_N^j]^T$ . The analysis of stability of the used method can be achieved if we assume that

$$\beta_i^j = h(j)e^{m_x x_i}. \tag{8.4.5}$$

For simplicity, we first assume that the value of  $\beta$  is unity and then substitute (8.4.5) in (8.4.4) so that the Caputo–Fabrizio derivative

$${}_0^C \mathcal{D}_x^\alpha f(x) = \frac{M(\alpha)}{1-\alpha} \int_0^x \frac{df(t)}{dt} \exp \left[ -\alpha \frac{x-t}{1-\alpha} \right] dt$$

becomes

$$\begin{aligned}
& \omega(j+1) \left( 8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + u_\alpha \mu_{n,j,j} + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \\
& = \omega(j) \left( -8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \\
& \quad + \sum_{k=1}^{j-1} (g_{n,j,k} p_\alpha - u_\alpha \mu_{n,j,k}) \omega(k+1) - p_\alpha \sum_{k=1}^{j-1} \omega(k) g_{n,j,k}. \tag{8.4.6}
\end{aligned}$$

If  $1 < j$ , the part with summation results in zero; therefore, with  $0 = j$ , Eq. (8.4.6) yields

$$\begin{aligned}
& \omega(1) \left( 8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + u_\alpha \mu_{n,j,j} + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \\
& = \omega(0) \left( -8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right). \tag{8.4.7}
\end{aligned}$$

Then, rearranging and applying the absolute value on both sides of above equation, we have

$$\left| \frac{\omega(1)}{\omega(0)} \right| = \left| \frac{(-8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR)}{(8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + u_\alpha \mu_{n,j,j} + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR)} \right| < 1, \tag{8.4.8}$$

which shows that

$$\left| \frac{\omega(1)}{\omega(0)} \right| < 1.$$

**Theorem 8.4.1** *If  $\omega(j)$  is the solution of Eq. (8.4.6), then, for every integer  $j \geq 1$ , the following relation holds:*

$$\omega(j) < \omega(0). \quad (8.4.9)$$

*Proof* We employ the recursive technique on the natural number  $j$  to achieve this proof. Further, we verify the proof for  $j = 0$ , as above. Next, we assume that for any  $k > 1$ , the inequality holds, then, for  $k = j$ , we have the following:

$$\begin{aligned} \omega(j) & \left( -8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + u_\alpha \mu_{n,j,j} + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \\ & = \omega(j-1) \left( 8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \\ & \quad + \sum_{k=1}^{j-1} (g_{n,j,k} p_\alpha - u_\alpha \mu_{n,j,k}) \omega(k+1) - p_\alpha \sum_{k=1}^{j-1} \omega(k) g_{n,j,k}. \end{aligned} \quad (8.4.10)$$

We apply the norm on both sides of the above equation to obtain the following result:

$$\begin{aligned} & \left\| \omega(j) \left( -8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + u_\alpha \mu_{n,j,j} + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right\| \\ & \leq \left\| \omega(j-1) \left( 8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right\| \\ & \quad + \left\| \sum_{k=1}^{j-1} (g_{n,j,k} p_\alpha - u_\alpha \mu_{n,j,k}) \omega(k+1) - p_\alpha \sum_{k=1}^{j-1} \omega(k) g_{n,j,k} \right\|. \end{aligned} \quad (8.4.11)$$

By employing the triangular equality and other useful properties, we have

$$\begin{aligned} & \|\omega(j)\| \left\| \left( 8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + u_\alpha \mu_{n,j,j} + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right\| \\ & \leq |\omega(j-1)| \left\| \left( -8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right\| \\ & \quad + \|\omega(k+1)\| \sum_{k=1}^{j-1} |g_{n,j,k} p_\alpha - u_\alpha \mu_{n,j,k}| + |p_\alpha| \sum_{k=1}^{j-1} \|\omega(k)\| |g_{n,j,k}|. \end{aligned} \quad (8.4.12)$$

By using the recursive, we obtain

$$\begin{aligned}
 & \|\omega(j)\| \left| \left( 8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + u_\alpha \mu_{n,j,j} + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right| \\
 & < |\omega(0)| \left\| \left( -8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right\| \\
 & \quad + \|\omega(0)\| \sum_{k=1}^{j-1} |g_{n,j,k} p_\alpha - u_\alpha \mu_{n,j,k}| + |p_\alpha| \sum_{k=1}^{j-1} |g_{n,j,k}| \|\omega(0)\| \\
 & \|\omega(0)\| \left\{ \left\| \left( -8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right\| \right. \\
 & \quad \left. + \sum_{k=1}^{j-1} |g_{n,j,k} p_\alpha - u_\alpha \mu_{n,j,k}| + |p_\alpha| \sum_{k=1}^{j-1} |g_{n,j,k}| \right\}. \tag{8.4.13}
 \end{aligned}$$

Then

$$\frac{\|\omega(j)\|}{\|\omega(0)\|} < \frac{\left\{ \left\| \left( -8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right\| + \mathfrak{P} \right\}}{\left| \omega(j+1) \left( 8 \sin^2 \left( \frac{m_x x_i}{2} \right) \nu_1 + u_\alpha \mu_{n,j,j} + p_\alpha g_{n,j,j} + 2 \sin^2 \left( \frac{m_x x_i}{2} \right) GR \right) \right|} \leq 1, \tag{8.4.14}$$

where

$$\mathfrak{P} = \sum_{k=1}^{j-1} |g_{n,j,k} p_\alpha - u_\alpha \mu_{n,j,k}| + |p_\alpha| \sum_{k=1}^{j-1} |g_{n,j,k}|.$$

Thus,

$$\frac{\|\omega(j)\|}{\|\omega(0)\|} < 1.$$

The proof is completed. □

### 8.5 Application of the Caputo–Fabrizio Derivative in Caputo Sense to Time-Fractional Advection–Diffusion Equation

Here, we shall use the Caputo–Fabrizio derivative in the sense of Caputo and present a numerical solution for the time-fractional advection–diffusion equation in heterogeneous medium.

The reason for this modification is far-fetched from the fact that the fractional derivatives are recollection operational which recurrently distinguish indulgence of force or damage in the passable as in the case of inelastic media, or reconsideration of the porosity in the thinning out in permeable media and supplementary in comprehensive they are in traditional values throughout the subsequent theory of hydrology [5–7]. They are accredited not just for the motivation that they match appropriately a variety of noticeable actuality, nevertheless, in addition to the motive that they own the well-designed alongside with scrupulous property that although the order

of differentiation is integer, and they match by means of the classical derivative of that order. On the other hand, this chattel is not known only to the effect they characterize in the physical observable fact and conjectures if applying other differential operators, probably simpler nevertheless devoid of this property, one may get similar response of fractional-order derivative. Therefore, in order to well mimic the flow of the particles via porous media in different scales in the medium, the ordinary derivative in time is replaced with the scaled time-fractional derivative proposed by Caputo and Fabrizio in the sense of Caputo, as discussed in the previous chapter.

The equation under consideration here is

$${}^{\text{CF}}\mathcal{D}_t^\alpha (U(x, t)) = \frac{\theta}{\kappa_\delta} \frac{\partial^2 U(x, t)}{\partial x^2} - \frac{\omega p}{\kappa_\delta} \frac{\partial U(x, t)}{\partial x} + \frac{F(x, t)}{\kappa_\delta}, \quad (8.5.1)$$

where the four terms in (8.5.1) denote transient, advection–diffusion and source term,  $U(x, t)$  represents the heat, particle, pollution or any other physical quantities,  $\kappa$  is the specific of heat, particle, pollution or any other physical quantities,  $p$  is a positive parameter,  $\omega$  stands for the porosity, that is, the ratio of the liquid volume to the total volume of the medium through which the flow is taken place, parameters  $\delta$  and  $\theta$ , respectively, represent the mass density and thermal conductivity, and  $F(x, t)$  accounts for the source or nonlinear term.

By using previously defined scheme in (8.5.1), we have

$$\begin{aligned} \frac{M(\alpha)}{2\alpha} \sum_{k=1}^{j+1} \frac{U_i^k - U_i^{k-1}}{\xi} \left\{ \operatorname{erf} \left( (j-k) \frac{\alpha k}{1-\alpha} \right) - \operatorname{erf} \left( (j-k+1) \frac{\alpha k}{1-\alpha} \right) \right\} \\ = \frac{\theta}{2h^2 \kappa_\delta} \left\{ (U_{i+1}^{j+1} - 2U_i^{j+1} + U_{i-1}^{j+1}) + (U_{i+1}^j - 2U_i^j + U_{i-1}^j) \right\} \\ - \frac{\omega p}{\kappa_\delta} \left\{ (U_{i+1}^{j+1} - U_{i-1}^{j+1}) + (U_{i+1}^j - U_{i-1}^j) \right\} + \frac{F_i^{j+1} + F_i^j}{2\kappa_\delta}. \end{aligned} \quad (8.5.2)$$

Equation (8.5.2) can be converted to

$$\begin{aligned} \frac{M(\alpha)}{2\alpha} \left( \frac{U_i^{j+1} - U_i^j}{\xi} + \frac{U_i^{j+1-k} - U_i^{j-k}}{\xi} \right) d_{j,k}^\alpha \\ = \frac{\theta}{2h^2 \kappa_\delta} \left\{ (U_{i+1}^{j+1} - 2U_i^{j+1} + U_{i-1}^{j+1}) + (U_{i+1}^j - 2U_i^j + U_{i-1}^j) \right\} \\ - \frac{\omega p}{4h\kappa_\delta} \left\{ (U_{i+1}^{j+1} - U_{i-1}^{j+1}) + (U_{i+1}^j - U_{i-1}^j) \right\} + \frac{F_i^{j+1} + F_i^j}{2\kappa_\delta}. \end{aligned} \quad (8.5.3)$$

For the sake of simplicity, we put

$$u = \frac{M(\alpha)}{2\alpha\xi}, \quad v = \frac{\theta}{2h^2 \kappa_\delta}, \quad w = \frac{\omega p}{4h\kappa_\delta}.$$

By rearranging, we have the following recursive formula:

$$\begin{aligned} (ud_{j,k}^\alpha + 2v) U_i^{j+1} &= (ud_{j,k}^\alpha - 2v) U_i^j + u \sum_{k=1}^j (U_i^{j+1-k} - U_i^{j-k}) d_{j,k}^\alpha \\ &+ v \left\{ (U_{i+1}^{j+1} + U_{i-1}^{j+1}) + (U_{i+1}^j + U_{i-1}^j) \right\} - w \left\{ (U_{i+1}^{j+1} - U_{i-1}^{j+1}) + (U_{i+1}^j - U_{i-1}^j) \right\} \\ &+ \frac{F_i^{j+1} + F_i^j}{2\kappa_\delta}. \end{aligned} \quad (8.5.4)$$

### 8.5.1 Stability Analysis of the Numerical Method with the Caputo–Fabrizio Derivative for Caputo Type

We present in this section the stability analysis of the Crank–Nicholson scheme for time-fractional advection–diffusion equation. For this, we let  $c_i^j = U_i^j - u_i^j$  with  $u_i^j$  the approximate solution to  $U_i^j$  at the point  $(x_i, t_j)$  for  $i = 1, 2, \dots, M$  and, as usual the vector,  $c^j = [c_1^j, c_2^j, \dots, c_N^j]^T$ . The computational error committed while solving the time-fractional advection–diffusion equation with the Crank–Nicholson scheme is given as

$$\begin{aligned} (ud_{j,k}^\alpha + 2v) c_i^{j+1} &= (ud_{j,k}^\alpha - 2v) c_i^j + u \sum_{k=1}^j (c_i^{j+1-k} - c_i^{j-k}) d_{j,k}^\alpha \\ &+ v \left\{ (c_{i+1}^{j+1} + c_{i-1}^{j+1}) + (c_{i+1}^j + c_{i-1}^j) \right\} - w \left\{ (c_{i+1}^{j+1} - c_{i-1}^{j+1}) + (c_{i+1}^j - c_{i-1}^j) \right\} \\ &+ \frac{F_i^{j+1} + F_i^j}{2\kappa_\delta}. \end{aligned} \quad (8.5.5)$$

Let us assume that

$$c_i^j = f(j) \exp(\xi \sigma i j), \quad (8.5.6)$$

where  $\sigma$  is the real spatial wave number [8]. However, substituting Eq. (8.5.6) into (8.5.5), we obtain, for  $j = 0$ ,

$$\left( ud_{k,0}^\alpha + 4v \sin^2 \left( \frac{\sigma i}{2} \right) \right) f(1) = \left( ud_{k,0}^\alpha - 4v \sin^2 \left( \frac{\sigma i}{2} \right) \right) f(0),$$

and for  $j > 0$ , we obtain

$$\left(ud_{k,j}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)\right) f(j) = \left(ud_{k,j}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right) f(j-1) - u \sum_{s=1}^{j-1} f(j-s)d_{k,j}^\alpha + f(j+1)d_{k,0}^\alpha.$$

**Theorem 8.5.1** Assume that  $f(k)$  holds for the following equations:

$$\left(ud_{k,0}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)\right) f(1) = \left(ud_{k,0}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right) f(0), \quad (8.5.7)$$

and

$$\left(ud_{k,j}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)\right) f(j) = \left(ud_{k,j}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right) f(j-1) - u \sum_{s=1}^{j-1} f(j-s)d_{k,j}^\alpha + f(j+1)d_{k,0}^\alpha. \quad (8.5.8)$$

Then, for all  $k > 0$ ,

$$|f(j)| \leq |f(0)|. \quad (8.5.9)$$

*Proof* To prove the above theorem, we start by employing the recursive method on the natural number  $j$ . When  $j = 0$ , we obtain (8.5.8) which is formulated as follows:

$$\left|\frac{f(1)}{f(0)}\right| = \left|\frac{\left(ud_{k,0}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right)}{\left(ud_{k,0}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)\right)}\right| \leq 1. \quad (8.5.10)$$

□

This shows that

$$|f(1)| \leq |f(0)|.$$

The property is examined for  $j = 0$ . Let us assume that this property also holds for any  $j \geq 1$ . We shall verify in what follows if the property is also satisfied for  $j + 1$ :

$$\left(ud_{k,j}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)\right) f(j+1) = \left(ud_{k,j}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right) f(j) - u \sum_{s=1}^j f(j-s)d_{k,s}^\alpha. \quad (8.5.11)$$

Now taking into account the norms of both sides of Eq. (8.5.11), we get

$$\left|ud_{k,j}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)\right| |f(j+1)| \leq \left|ud_{k,j}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right| |f(j)| + \sum_{s=1}^j |f(j-s)| d_{k,s}^\alpha.$$

Nonetheless, we recall that the property satisfies up to  $j$ . Thus, the above equation is transformed into

$$\left|ud_{k,j}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)\right| |f(j+1)| \leq \left|ud_{k,j}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right| |f(0)| + \sum_{s=1}^j |f(0)| d_{k,s}^\alpha.$$

By rearranging, yields

$$\begin{aligned} &\left|ud_{k,j}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)\right| |f(j+1)| && (8.5.12) \\ &\leq \left\{ \left|ud_{k,j}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right| + \left\{ \operatorname{erf}\left[\frac{m\alpha i}{1-\alpha}\right] - \operatorname{erf}\left[\frac{\alpha i}{1-\alpha}\right] \right\} \right\} |f(0)|. \end{aligned}$$

It is important to note that

$$|\operatorname{erf}[x]| \leq 1, \quad \operatorname{erf}\left[\frac{m\alpha i}{1-\alpha}\right] - \operatorname{erf}\left[\frac{\alpha i}{1-\alpha}\right] \leq 0.$$

Therefore,

$$\frac{|f(j+1)|}{|f(0)|} \leq \frac{\left|ud_{k,j}^\alpha - 4v \sin^2\left(\frac{\sigma i}{2}\right)\right| + \left\{ \operatorname{erf}\left[\frac{m\alpha i}{1-\alpha}\right] - \operatorname{erf}\left[\frac{\alpha i}{1-\alpha}\right] \right\}}{ud_{k,j}^\alpha + 4v \sin^2\left(\frac{\sigma i}{2}\right)} \leq 1.$$

Then

$$\frac{|f(j+1)|}{|f(0)|} \leq 1.$$

According to the inductive technique, the property also satisfies for  $j + 1$  and any natural number. This completes the proof. The above theorem shows that the Crank–Nicholson scheme is stable for the advection–diffusion equation with the time-fractional Caputo–Fabrizio derivative in the sense of Caputo.

### 8.5.2 Convergence Analysis of the Numerical Scheme with the Caputo–Fabrizio Derivative for Caputo Type

Let us assume that the exact solution of our equation at the point  $(x_i, t_j)$  is  $U(x_i, t_j)$  for  $i = 1, 2, \dots, N$  and  $j = 1, 2, \dots, M$ . We also suppose that the difference between the exact and approximate solutions at that particular point is given by  $\nabla_i^j = U(x_i, t_j) - U_i^j$ , and the associated transpose matrix  $\nabla_i^j = U(x_i, t_j) - U_i^j$  for  $i = 0, 1, 2, \dots, N$  and  $j = 0, 1, 2, \dots, M$  is  $[\nabla_1^j, \nabla_2^j, \dots, \nabla_N^j]^T$ . However, the row  $\nabla^0$  is zero due to the fact that it denotes the initial condition. The recursive relation

in connection with the Crank–Nicholson scheme for the time-fractional advection–diffusion equation is given as

$$\begin{aligned} & \left(ud_{k,0}^\alpha + 2v\right) \nabla_i^1 + (w - v) \left(\nabla_{i+1}^1 + \nabla_{i-1}^1\right) - \frac{F_i^1 - F_i^0}{2\kappa_\delta} = \mathcal{E}_i^1, \quad j = 0, \quad (8.5.13) \\ & \left(ud_{k,0}^\alpha + 2v\right) \nabla_i^{j+1} - \left(ud_{i,j}^\alpha + 2v\right) \nabla_i^j + (w - v) \left(\nabla_{i+1}^{j+1} + \nabla_{i-1}^{j+1}\right) \\ & + (w - v) \left(\nabla_{i+1}^j + \nabla_{i-1}^j\right) - \frac{F_i^{j+1} - F_i^j}{2\kappa_\delta} = -u \sum_{s=1}^{j-1} \nabla_i^{j-1} d_{i,s}^\alpha + \mathcal{E}_i^{j+1}, \quad j > 0, \end{aligned}$$

with the remainder term given as

$$\begin{aligned} \mathcal{E}_i^{j+1} &= uU(x_i, t_{j+1})d_{i,s}^\alpha + u \sum_{s=1}^j v(x_i, t_{j-s})d_{i,s}^\alpha \\ &- v \left\{ \left( U(x_{i+1}, t_{j+1}) - 2U(x_i, t_{j+1}) + U(x_{i-1}, t_{j+1}) \right) \right. \\ &+ \left. \left( U(x_{i+1}, t_j) - 2U(x_i, t_j) + U(x_{i-1}, t_j) \right) \right\} + w \left\{ \left( U(x_{i+1}, t_{j+1}) + U(x_{i-1}, t_{j+1}) \right) \right. \\ &\times \left. \left( U(x_{i+1}, t_j) + U(x_{i-1}, t_j) \right) \right\} - \frac{F_i^{j+1} - F_i^j}{2\kappa_\delta}. \quad (8.5.14) \end{aligned}$$

By using the full approximation and considering the remaining terms, we have the following relation:

$$\mathcal{E}_i^{j+1} \leq D(2k + h^2).$$

Hence, we conclude with the following theorem.

**Theorem 8.5.2** *The Crank–Nicolson scheme for the advection–diffusion equation with time-fractional Caputo–Fabrizio derivative in Caputo sense converges, and there exists a positive constant  $D$  such that*

$$\|U(x_i, t_i) - U_i^j\| \leq D(2k + h^2) \quad \text{for all } i = 0, 1, 2, \dots, M \text{ and } j = 1, 2, \dots, N.$$

## 8.6 Applications of Fractional Derivatives to Diffusion–Advection Equation

Consider the diffusion–advection problem

$${}_0\mathbf{D}_x^2 U(x, t) + \frac{\nu}{d} {}_0\mathbf{D}_x U(x, t) + \frac{1}{d} {}_0\mathbf{D}_t U(x, t) = 0, \quad (8.6.1)$$

where  $U$  is the concentration,  $d$  is the diffusion coefficient and  $\nu$  denotes the drift velocity; this equation is considered only in one-dimensional space.

In this section, we present numerical approximations of the diffusion–advection problem (8.6.1) involving operators of type Riemann–Liouville, Caputo–Fabrizio–Riemann and Atangana–Baleanu in Riemann–Liouville sense.

### 8.6.1 Riemann–Liouville Approach

With the Riemann–Liouville operator, the above diffusion–advection equation is given as

$${}^RL\mathbf{D}_x^\beta U(x, t) + \frac{1}{d} \left( \nu {}^RL\mathbf{D}_x^\varphi U(x, t) + {}^RL\mathbf{D}_t^\alpha U(x, t) \right) = 0, \quad 1 < \beta \leq 2, \quad 0 < \varphi \leq 1, \quad 0 < \alpha \leq 1. \quad (8.6.2)$$

The numerical approximation of (8.6.2) is

$$\begin{aligned} & \frac{(\Delta x)^{-1-\beta}}{2\Gamma(2-\varphi)} \left[ \sum_{k=0}^j u(x_{k+1}) f_{j,k}^\beta - 2 \sum_{k=0}^{j-1} u(x_{k+1}) f_{j,k}^{\beta,1} + \sum_{k=0}^{j-1} u(x_{k+1}) f_{j,k}^{\beta,2} \right] + W_{\beta,j,k} \\ & + \frac{\nu}{d} \left\{ \frac{1}{\Delta x \Gamma(2-\varphi)} \left[ \sum_{k=0}^j \frac{u(x_{k+1}) + u(x_k)}{2} \left[ (x_{j+1} - x_{k+1}^{1-\varphi}) - (x_{j+1} - x_k)^{1-\varphi} \right] \right] \right. \\ & \left. - \sum_{k=1}^j \frac{u(x_k) + u(x_{k-1})}{2} \left[ (x_j - x_{k+1})^{1-\varphi} \right] + W_{\alpha,j} \right\} \\ & = -\frac{1}{d} \left\{ \frac{1}{\Delta t \Gamma(2-\alpha)} \cdot \left[ \sum_{k=0}^j \frac{u(t_{k+1}) + u(t_k)}{2} \left[ (t_{j+1} - t_{k+1})^{1-\alpha} - (t_{j+1} - t_k)^{1-\alpha} \right] \right] \right. \\ & \left. - \sum_{k=1}^j \frac{u(t_k) + u(t_{k-1})}{2} \left[ (t_j - t_{k+1})^{1-\alpha} - (t_j - t_k)^{1-\alpha} \right] + W_{\alpha,j} \right\}, \quad (8.6.3) \end{aligned}$$

where

$$\begin{aligned} W_{\varphi,j,k} &= \frac{(\Delta x)^{-2}}{2\Gamma(2-\varphi)} \left[ \sum_{k=0}^j \int_{x_k}^{x_{k+1}} \frac{u(r) - u(x_{k+1})}{(x_{j+1} - r)^{\varphi-1}} dr \right. \\ & \left. - 2 \sum_{k=0}^{j-1} \int_{x_k}^{x_{k+1}} \frac{u(r) - u(x_{k+1})}{(x_j - r)^{\varphi-1}} dr + \sum_{k=1}^{j-1} \int_{x_k}^{x_{k+1}} \frac{u(r) - u(x_{k+1})}{(x_{j-1} - r)^{\varphi-1}} dr \right], \\ f_{j,k}^\varphi &= (j-k)^{1-\varphi} - (j-k+1)^{1-\varphi}, \\ f_{j,k}^{\varphi,1} &= (j-k-1)^{1-\varphi} - (j-k)^{1-\varphi}, \\ f_{j,k}^{\varphi,2} &= (j-k-2)^{1-\varphi} - (j-k-1)^{1-\varphi}, \end{aligned}$$

$$W_{\varphi,j} = \frac{1}{\Delta x \Gamma(1-\varphi)} \left\{ \sum_{k=0}^j \int_{x_k}^{x_{k+1}} \frac{u(r) - u(x_{k+1})}{(x_{j+1} - r)^\varphi} dr - \sum_{k=0}^{j-1} \int_{x_k}^{x_{k+1}} \frac{u(r) - u(x_{k+1})}{(x_j - r)^\varphi} dr \right\}$$

$$W_{\alpha,j} = \frac{1}{\Delta t \Gamma(1-\alpha)} \left\{ \sum_{k=0}^j \int_{t_k}^{t_{k+1}} \frac{u(r) - u(t_{k+1})}{(t_{j+1} - r)^\alpha} dr - \sum_{k=0}^{j-1} \int_{t_k}^{t_{k+1}} \frac{u(r) - u(t_{k+1})}{(t_j - r)^\alpha} dr \right\}.$$

### 8.6.2 Caputo–Fabrizio–Riemann Approach

The numerical approximation of the fractional diffusion–advection equation via Caputo–Fabrizio–Riemann operator is given by

$${}_0^{CFR} \mathbf{D}_x^\beta U(x, t) + \frac{1}{d} \left( {}_0^{CFR} \mathbf{D}_x^\varphi U(x, t) + {}_0^{CFR} \mathbf{D}_t^\alpha U(x, t) \right) = 0, \\ 1 < \beta \leq 2, \quad 0 < \varphi \leq 1, \quad 0 < \alpha \leq 1. \quad (8.6.4)$$

The numerical approximation of (8.6.4) is

$$\frac{1}{2(\Delta x)^2} \left[ \sum_{k=0}^j \frac{u(x_{k+1})}{2} g_{j,k}^{\beta,1} - 2 \sum_{k=0}^{j-1} \frac{u(x_{k+1})}{2} g_{j,k}^{\beta,2} + \sum_{k=0}^j \frac{u(x_{k+1})}{2} g_{j,k}^{\beta,3} \right] + G \\ + \frac{\nu}{d} \left\{ \frac{M(\varphi)}{\Delta x(\varphi)} \left[ \sum_{k=0}^j \frac{u(x_{k+1}) + u(x_k)}{2} \exp\left(-\varphi \frac{x_{j+1} - x_{k+1}}{1-\varphi}\right) - \exp\left(-\varphi \frac{x_{j+1} - x_k}{1-\varphi}\right) \right. \right. \\ \left. \left. - \sum_{k=1}^j \frac{u(x_k) + u(x_{k-1})}{2} \exp\left(-\varphi \frac{x_j - x_{k+1}}{1-\varphi}\right) - \exp\left(-\varphi \frac{x_j - x_k}{1-\varphi}\right) + V_{\varphi,j,k} \right] \right\} \\ = -\frac{1}{d} \left\{ \frac{M(\alpha)}{\Delta t(\alpha)} \cdot \left[ \sum_{k=0}^j \frac{u(t_{k+1}) + u(t_k)}{2} \exp\left(-\alpha \frac{t_{j+1} - t_{k+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_{j+1} - t_k}{1-\alpha}\right) \right. \right. \\ \left. \left. - \sum_{k=1}^j \frac{u(t_k) + u(t_{k-1})}{2} \exp\left(-\alpha \frac{t_j - t_{k+1}}{1-\alpha}\right) - \exp\left(-\alpha \frac{t_j - t_k}{1-\alpha}\right) \right] + V_{\alpha,j,k} \right\}, \quad (8.6.5)$$

where

$$g_{j,k}^{\beta,1} = \operatorname{erfc} \left\{ -\beta \frac{x_{j+1} - x_{k+1}}{1-\beta} \right\} - \operatorname{erfc} \left\{ -\beta \frac{x_{j+1} - x_k}{1-\beta} \right\}, \\ g_{j,k}^{\beta,2} = \operatorname{erfc} \left\{ -\beta \frac{x_j - x_{k+1}}{1-\beta} \right\} - \operatorname{erfc} \left\{ -\beta \frac{x_j - x_k}{1-\beta} \right\}, \\ g_{j,k}^{\beta,3} = \operatorname{erfc} \left\{ -\beta \frac{x_{j-1} - x_{k+1}}{1-\beta} \right\} - \operatorname{erfc} \left\{ -\beta \frac{x_{j-1} - x_k}{1-\beta} \right\},$$

$$G = \frac{\alpha}{(1-\beta)\sqrt{\pi}} \left\{ \sum_{k=0}^j \int_{x_k}^{x_{k+1}} (u(\xi) - u(x_{j+1})) \exp\left(-\left(\frac{\beta}{1-\beta}\right)^2 (x_{j+1} - \xi)^2\right) d\xi \right. \\ \left. - 2 \sum_{k=0}^{j-1} \int_{x_k}^{x_{k+1}} (u(\xi) - u(x_{j+1})) \exp\left(-\left(\frac{\beta}{1-\beta}\right)^2 (x_j - \xi)^2\right) d\xi \right. \\ \left. + \sum_{k=1}^{j-1} \int_{x_k}^{x_{k+1}} (u(\xi) - u(x_{j+1})) \exp\left(-\left(\frac{\beta}{1-\beta}\right)^2 (x_{j-1} - \xi)^2\right) d\xi \right\},$$

$$V_{\varphi,j,k} = \frac{M(\varphi)}{(1-\varphi)\Delta x} \left\{ \sum_{k=0}^j \int_{x_k}^{x_{k+1}} \{u(r) - u(x_{k+1})\} \exp\left(-\frac{\varphi}{1-\varphi}(x_{j+1} - \phi)\right) dr \right. \\ \left. - \sum_{k=0}^{j-1} \int_{x_k}^{x_{k+1}} \{u(r) - u(x_{k+1})\} \exp\left(-\frac{\varphi}{1-\varphi}(x_j - \phi)\right) dr \right\},$$

similarly

$$V_{\alpha,j,k} = \frac{M(\alpha)}{(1-\alpha)\Delta t} \left\{ \sum_{k=0}^j \int_{t_k}^{t_{k+1}} \{u(r) - u(t_{k+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_{j+1} - \phi)\right) dr \right. \\ \left. - \sum_{k=0}^{j-1} \int_{t_k}^{t_{k+1}} \{u(r) - u(t_{k+1})\} \exp\left(-\frac{\alpha}{1-\alpha}(t_j - \phi)\right) dr \right\},$$

the  $\operatorname{erfc}\{\cdot\}$  represents the error function.

### 8.6.3 Atangana–Baleanu–Riemann Approach

The numerical approximation of the fractional diffusion–advection equation via Atangana–Baleanu–Riemann operator is given by

$${}^{\text{ABR}}\mathbf{D}_x^\beta U(x, t) + \frac{1}{d} \left( {}^{\text{ABR}}\mathbf{D}_x^\varphi U(x, t) + {}^{\text{ABR}}\mathbf{D}_t^\alpha U(x, t) \right) = 0, \\ 1 < \beta \leq 2, \quad 0 < \varphi \leq 1, \quad 0 < \alpha \leq 1. \quad (8.6.6)$$

The numerical approximation of (8.6.4) is

$$\begin{aligned}
& \frac{1}{2(\Delta x)^2} \left\{ \sum_{k=0}^j \frac{u(x_{k+1})}{2} e_{j,k}^{\beta,1} - 2 \sum_{k=0}^{j-1} \frac{u(x_{k+1})}{2} e_{j,k}^{\beta,2} + \sum_{k=0}^j \frac{u(x_{k+1})}{2} e_{j,k}^{\beta,3} \right\} + V \\
& + \frac{\nu}{d} \left\{ \frac{AB(\varphi)}{\Delta x(1-\varphi)} \left[ \sum_{k=0}^j \frac{u(x_{k+1}) + u(x_k)}{2} \Psi_j^{\varphi,1} - \frac{AB(\varphi)}{1-\varphi} \sum_{k=0}^{j-1} \frac{u(x_{k+1}) + u(x_k)}{2} \Psi_j^{\varphi,2} \right] + Q_j^\varphi \right\} \\
& = -\frac{1}{d} \left\{ \frac{AB(\alpha)}{\Delta t(1-\alpha)} \left[ \sum_{k=0}^j \frac{u(t_{k+1}) + u(t_k)}{2} \Phi_j^{\alpha,1} - \frac{AB(\alpha)}{1-\alpha} \sum_{k=0}^{j-1} \frac{u(t_{k+1}) + u(t_k)}{2} \Phi_j^{\alpha,2} \right] + P_j^\alpha \right\},
\end{aligned}$$

where

$$\begin{aligned}
e_{j,k}^{\beta,1} &= E_{\beta,2} \left\{ -\beta \frac{x_{j+1} - x_{k+1}}{1-\beta} \right\} - E_{\beta,2} \left\{ -\beta \frac{x_{j+1} - x_k}{1-\beta} \right\}, \\
e_{j,k}^{\beta,2} &= E_{\beta,2} \left\{ -\beta \frac{x_j - x_{k+1}}{1-\beta} \right\} - E_{\beta,2} \left\{ -\beta \frac{x_j - x_k}{1-\beta} \right\}, \\
e_{j,k}^{\beta,3} &= E_{\beta,2} \left\{ -\beta \frac{x_{j-1} - x_{k+1}}{1-\beta} \right\} - E_{\beta,2} \left\{ -\beta \frac{x_{j-1} - x_k}{1-\beta} \right\},
\end{aligned}$$

$$\begin{aligned}
V &= \frac{\alpha}{(1-\beta)\sqrt{\pi}} \left\{ \sum_{k=0}^j \int_{x_k}^{x_{k+1}} (u(\tau) - u(x_{j+1})) E_{\beta,2} \left( -\left(\frac{\beta}{1-\beta}\right)^2 (x_{j+1} - \tau)^2 \right) d\tau \right. \\
& - 2 \sum_{k=0}^{j-1} \int_{x_k}^{x_{k+1}} (u(\tau) - u(x_{j+1})) E_{\beta,2} \left( -\left(\frac{\beta}{1-\beta}\right)^2 (x_j - \tau)^2 \right) d\tau \\
& \left. + \sum_{k=1}^{j-1} \int_{x_k}^{x_{k+1}} (u(\tau) - u(x_{j+1})) E_{\beta,2} \left( -\left(\frac{\beta}{1-\beta}\right)^2 (x_{j-1} - \tau)^2 \right) d\tau \right\},
\end{aligned}$$

$$\begin{aligned}
\Psi_j^{\varphi,1} &= \int_{x_k}^{x_{k+1}} E_\varphi \left[ -\frac{\varphi}{1-\varphi} (x_{j+1} - \zeta)^\varphi \right] = (x_{j+1} - x_{k+1}) E_{\varphi,2} \left[ -\frac{\varphi}{1-\varphi} (x_{j+1} - x_{k+1})^\varphi \right] \\
& + (x_{j+1} - x_k) E_{\varphi,2} \left[ -\frac{\varphi}{1-\varphi} (x_{j+1} - x_k)^\varphi \right],
\end{aligned}$$

$$\begin{aligned}
\Psi_j^{\varphi,2} &= \int_{x_k}^{x_{k+1}} E_\varphi \left[ -\frac{\varphi}{1-\varphi} (x_j - \zeta)^\varphi \right] = (x_j - x_{k+1}) E_{\varphi,2} \left[ -\frac{\varphi}{1-\varphi} (x_j - x_{k+1})^\varphi \right] \\
& + (x_j - x_k) E_{\varphi,2} \left[ -\frac{\varphi}{1-\varphi} (x_j - x_k)^\varphi \right],
\end{aligned}$$

$$\begin{aligned}
Q_{\varphi,j,k} &= \frac{M(\varphi)}{(1-\varphi)\Delta x} \left\{ \sum_{k=0}^j \int_{x_k}^{x_{k+1}} \{u(\xi) - u(x_{k+1})\} E_\varphi \left[ -\frac{\varphi}{1-\varphi} (x_{j+1} - \tau) \right] d\xi \right. \\
& \left. - \sum_{k=0}^{j-1} \int_{x_k}^{x_{k+1}} \{u(\xi) - u(x_{k+1})\} E_\varphi \left[ -\frac{\varphi}{1-\varphi} (x_j - \tau) \right] d\xi \right\},
\end{aligned}$$

$$\begin{aligned} \Phi_j^{\alpha,1} &= \int_{t_k}^{t_{k+1}} E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_{j+1} - \zeta)^\alpha \right] = (t_{j+1} - t_{k+1}) E_{\alpha,2} \left[ -\frac{\alpha}{1-\alpha} (t_{j+1} - t_{k+1})^\alpha \right] \\ &\quad + (t_{j+1} - t_k) E_{\alpha,2} \left[ -\frac{\alpha}{1-\alpha} (t_{j+1} - t_k)^\alpha \right], \end{aligned}$$

$$\begin{aligned} \Phi_j^{\alpha,2} &= \int_{t_k}^{t_{k+1}} E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_j - \zeta)^\alpha \right] = (t_j - t_{k+1}) E_{\alpha,2} \left[ -\frac{\alpha}{1-\alpha} (t_j - t_{k+1})^\alpha \right] \\ &\quad + (t_j - t_k) E_{\alpha,2} \left[ -\frac{\alpha}{1-\alpha} (t_j - t_k)^\alpha \right], \end{aligned}$$

$$\begin{aligned} P_{\alpha,j,k} &= \frac{M(\alpha)}{(1-\alpha)\Delta t} \left\{ \sum_{k=0}^j \int_{t_k}^{t_{k+1}} \{u(\xi) - u(t_{k+1})\} E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_{j+1} - \tau) \right] d\xi \right. \\ &\quad \left. - \sum_{k=0}^{j-1} \int_{t_k}^{t_{k+1}} \{u(\xi) - u(t_{k+1})\} E_\alpha \left[ -\frac{\alpha}{1-\alpha} (t_j - \tau) \right] d\xi \right\}. \end{aligned}$$

## 8.7 Application to Partial Fractional Differential Equation

This chapter deals with the application of some of the previously discussed fractional derivative operators (such as the Caputo, the Caputo–Fabrizio and the Atangana–Baleanu fractional derivatives) to model partial differential equations in both space and time. We intend to consider examples of one, two and multicomponent fractional reaction–diffusion equations.

Mathematically speaking, reaction–diffusion model takes the form of a semi-linear parabolic differential equation given as

$$u_t = D\Delta^2 u + \mathbf{N}(u), \quad (8.7.1)$$

where  $u(x, t)$  is the concentration of a substance- or vector-dependent variables,  $D$  is the diagonal matrix of diffusion coefficients,  $\Delta^2$  represents the Laplacian operator, often expressed as the second-order partial derivatives and  $\mathbf{N}(u)$  is a nonlinear reaction term that represents the local kinetics. Reaction–diffusion equation of the form (8.7.1) mathematically describes how the concentration of one or more substances are distributed in space, which change under the influence of two scenarios; the local chemical reactions in which the substances are transformed into each other, and diffusion ( $D$ ) which causes the substances to spread out over a surface in space ( $x$ ) and time  $t$ . In biological context, the solution of this type of equation has been used to study a wide range of behaviours, such as the formation of travelling waves, self-organized structures such as spots and stripes, or more intricate pattern like dissipative solitons [19, 31, 50, 58].

### 8.7.1 The Fisher Equation

For this example, we are interested in the application of the prototype reaction–diffusion equation [55, 58]

$$u_t = D\Delta^2 u + \beta u \left( 1 - \frac{u^\rho}{\kappa} \right), \quad t > 0, \tag{8.7.2}$$

where  $\rho > 0$ ,  $D$  remains as the diffusion coefficient,  $\beta$  is considered to be the growth rate,  $u$  is the species density,  $\kappa$  is the carrying capacity and  $\Delta^2$  is the Laplacian operator in one and higher dimensions, Eq.(8.7.2) has a long attention span history in the study of propagation phenomena such as flames distribution, migration of biological species or tumour growth, heat and mass transfer and ecology among many others. The time-dependent reaction–diffusion equation (8.7.2) was first considered by Fisher [19] in one dimension as a deterministic model for the spatial spread of a favoured gene in a population and it has since then applied to other fields like population dynamics, combustion theory and chemical kinetics. Applications of the Fisher equation have been extended to various fields of research, for instance, the logistic population growth models [11, 34, 47], flame propagation [26, 77] and the Brownian motion processes [9]. Analytical representations of travelling wave solutions for Fisher equation have been investigated in one dimension [1, 17, 20, 32, 36] and in two space dimensions [10]. The seminal and classical paper on this equation was reported by Kolmogorov et al. [31], with extensive discussion and references in the books by Britton [11], Fife [18], Kot [33] and Murray [48–51] among others.

The interests here is not in classical time-dependent equation, thus we are motivated by formulating the fractional version (8.7.2) in the form

$$\mathcal{D}_t^\alpha = D\Delta^2 + \beta u \left( 1 - \frac{u^\rho}{\kappa} \right), \quad 0 < \alpha < 1, \quad t > 0, \tag{8.7.3}$$

where  $\mathcal{D}_t^\alpha$  is the given time-fractional derivative of order  $\alpha$  which can be expressed in terms of the Caputo, Caputo–Fabrizio or the Atangana–Baleanu operators.

In what follows, we shall consider briefly the numerical integration of Eq.(8.7.3) in one and two spatial dimensions. We first apply the concept of method of lines [23, 61] for the spatial approximation of the derivatives in (8.7.3) by applying the central finite difference scheme. In one-dimensional space, we discretize the spatial domain with step size  $h = x/(N - 1)$  and approximate the second-order spatial derivative at the right-hand side of (8.7.3) using the fourth-order central finite difference scheme, which gives a system of nonlinear ordinary differential equations

$$\mathcal{D}_t^\alpha = D \left( \frac{-u_{i+2,j} + 16u_{i+1,j} - 30u_{i,j} + 16u_{i-1,j} - u_{i-2,j}}{12h^2} \right) + \beta u_{i,j} \left( 1 - \frac{(u_{i,j})^\rho}{\kappa} \right) \tag{8.7.4}$$

for  $i = 1, 2, \dots, N$  and  $u = [u_1^j, u_2^j, \dots, u_N^j]^T$ . Equation (8.7.4) is then solved subject to initial condition of the form  $u(x, t = 0) = u_0(x)$  for  $x \in [a, b]$ , and the zero-flux boundary conditions  $u_a = u_b = 0$ .

In two dimensions, the initial and boundary fractional Fisher equation becomes

$$\begin{aligned} \mathcal{D}_t^\alpha &= D(u_{xx} + u_{yy}) + \beta u \left(1 - \frac{u^\rho}{\kappa}\right), \quad (x, y) \in \Omega = (a \leq x, y \leq b), \quad t > 0, \\ u(x, y, 0) &= u_0(x, y), \quad a \leq x, y \leq b, \\ u(a, t) = u(b, t) &= 0, \quad t > 0, \quad 0 < \alpha < 1, \end{aligned} \tag{8.7.5}$$

by following the approach introduced in [58], we first discretize the spatial domain by mesh  $(x_i, y_j) = (a + i \times h_x, a + j \times h_y)$ , where  $h_x = (b - a)/(N_x + 1)$ ,  $h_y = (b - a)/(N_y + 1)$  and  $0 \leq i \leq N_x + 1$  and  $0 \leq j \leq N_y + 1$ . Using fourth-order central difference discretization on the diffusion, we obtain a system of nonlinear ODEs

$$\begin{aligned} \mathcal{D}_t^\alpha &= \frac{D}{12} \left[ \frac{-u_{i+2,j} + 16u_{i+1,j} - 30u_{i,j} + 16u_{i-1,j} - u_{i-2,j}}{h_x^2} \right] + \\ &\frac{D}{12} \left[ \frac{-u_{i,j+2} + 16u_{i,j+1} - 30u_{i,j} + 16u_{i,j-1} - u_{i,j-2}}{h_y^2} \right] + \\ &\beta u_{i,j} \left(1 - \frac{(u_{i,j})^\rho}{\kappa}\right), \end{aligned} \tag{8.7.6}$$

which in a more compact representation becomes

$$\mathcal{D}_t^\alpha = \mathbf{L}u + \mathbf{F}u, \tag{8.7.7}$$

where  $\mathbf{L}$  is regarded as the Toeplitz matrix representing the linear part and  $\mathbf{F}$  is a vector that contains the nonlinear function, and

$$u = \begin{pmatrix} u_{1,1} & u_{1,2} & \dots & u_{1,N_y} & u_{1,N_y+1} \\ u_{2,1} & u_{2,2} & \dots & u_{2,N_y} & u_{2,N_y+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ u_{N_x,1} & u_{N_x,2} & \dots & u_{N_x,N_y} & u_{N_x,N_y+1} \end{pmatrix}_{N_x \times N_y+1}. \tag{8.7.8}$$

Another efficient numerical spatial discretization technique that has been applied in conjunction with the time-stepping solvers, especially, the exponential time-differencing Runge–Kutta [27, 61] is the Fourier spectral method [75, 76]. With description adapted from, a brief discussion on the Fourier spectral method when applied to (8.7.5) will be [75, 76] presented. Given a periodic function  $u$  on the spatial grid  $x_j$ , the discrete Fourier transform (DFT) is defined as

$$\widehat{u}_k = h \sum_{j=i}^N e^{-ikx_j} u_j, \quad k = -\frac{N}{2} + 1, \dots, \frac{N}{2} \tag{8.7.9}$$

and the inverse DFT is defined by

$$u_j = \frac{1}{2\pi} \sum_{k=-N/2}^{N/2} e^{-ikx_j} \widehat{u}_k, \quad j = 1, 2, \dots, N, \quad (8.7.10)$$

where  $k$  is called the wave number. By applying this method to (8.7.5) with all the time stepping in Fourier space, it results in the following system of ODEs:

$$\widehat{\mathcal{D}}_t^\alpha = -Dk^2 \widehat{u} + \widehat{F(u)}, \quad (8.7.11)$$

so that the linear term of (8.7.5) has a diagonal representation. Next, the resulting system of ODEs can be advanced with any time-stepping integrator.

The Cox and Matthews fourth-order version of exponential time-differencing Runge–Kutta method [15] is given as

$$\begin{aligned} u_{n+1} = & u_n e^{\mathbf{L}h} + \mathbf{F}(u_n, t_n)[-4 - h\mathbf{L} + e^{\mathbf{L}h}(4 - 3h\mathbf{L} + h^2\mathbf{L}^2)] \\ & + 2((F)(a_n, t_n + h/2) + \mathbf{F}(b_n, t_n + h/2))[2 + h\mathbf{L} + e^{\mathbf{L}h}(-2 + h\mathbf{L})] \\ & + \mathbf{F}(c_n, t_n + h)[-4 - 3h\mathbf{L} - h^2\mathbf{L}^2 + e^{\mathbf{L}h}(4 - h\mathbf{L})]/h^2\mathbf{L}^3, \end{aligned} \quad (8.7.12)$$

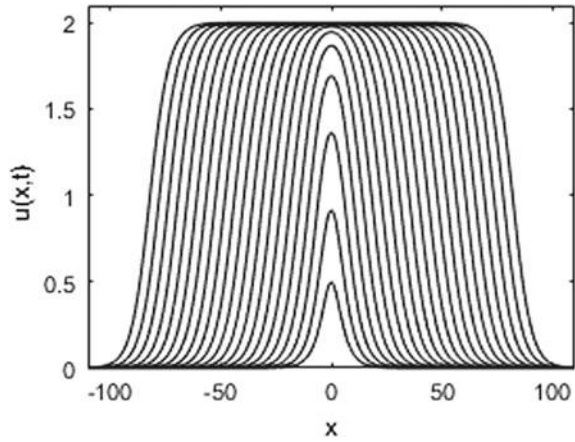
where

$$\begin{aligned} a_n &= u_n e^{\mathbf{L}h/2} + (e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{F}(u_n, t_n)/\mathbf{L}, \\ b_n &= u_n e^{\mathbf{L}h/2} + (e^{\mathbf{L}h/2} - \mathbf{I})\mathbf{F}(a_n, t_n + h/2)/\mathbf{L}, \\ c_n &= u_n e^{\mathbf{L}h/2} + (e^{\mathbf{L}h/2} - \mathbf{I})(2\mathbf{F}(b_n, t_n + h/2) - \mathbf{F}(u_n, t_n))/\mathbf{L}. \end{aligned} \quad (8.7.13)$$

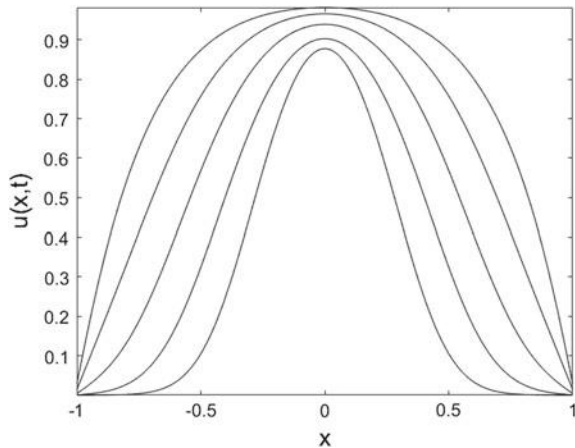
If (8.7.12) is used in conjunction with either of ODEs (8.7.7) or (8.7.11),  $\mathbf{L}$  represents the linear diffusion part, while  $\mathbf{F}$  stands for the nonlinear part. For detailed analysis on derivation and stability of this method, our readers are referred to Refs. [15, 27, 35, 61].

For all the numerical simulations performed in one and two dimensions, we let  $\Delta t = 0.25$ ,  $\Delta x = 0.25$  and  $N = 200$ . In Fig. 8.1, we present the contour plot of fraction Fisher equation with the Caputo–Fabrizio derivative of order  $\alpha$ . This result corresponds to the classical case obtained at  $\alpha = 1$ . Other parameters are given as  $D = 0.8$ ,  $\kappa = 1.66$ ,  $\beta = 1$ ,  $\rho = 2$  for final simulation time  $t = 1.0$ . Numerical propagation of system (8.7.3) for different  $\alpha$  values and spatial domain  $x \in [-L, L]$ , where  $L$  is chosen large enough to give room for the waves to propagate, is displayed in Figs. 8.2, 8.3, 8.4, 8.5, 8.6 and 8.7. It is evident in the displayed results that each solution gives a sinusoidal pattern with initial sharp peaks in the middle which disappear and get flatter as the fractional parameter  $\alpha$  is increasing (Figs. 8.8, 8.9 and 8.10). The contour plots in Figs. 8.11, 8.12, 8.13 and surface plot Fig. 8.14 show the approximate solution for the case  $\beta = 1$ ,  $\rho = 1$ ,  $\kappa = 1$  and  $D = 0.5$ , subject to initial condition

**Fig. 8.1** 1D contour plot (8.7.3) when  $\alpha = 1$  and  $t = 1.0$



**Fig. 8.2** 1D contour plot (8.7.3) when  $\alpha = 0.15$  and  $t = 1.0$  for  $L = 4$



$$u(x, 0) = \left[ 1 + \exp\left(\frac{\sqrt{6}}{6}x\right) \right]^{-2}. \tag{8.7.14}$$

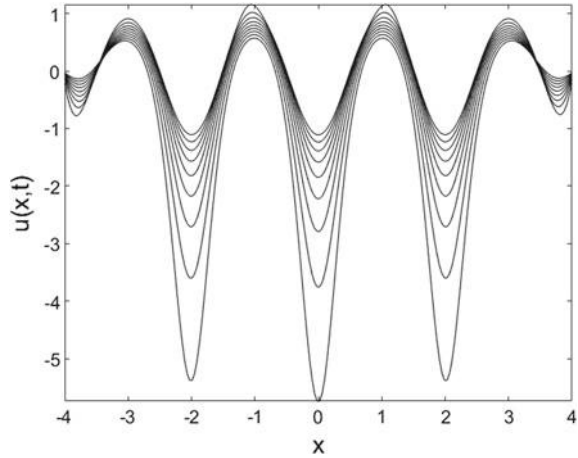
In Figs. 8.15, 8.16 and 8.17, we apply the Caputo fractional derivative by setting  $\mathcal{D}_t^\alpha = {}^C_0\mathcal{D}_t^\alpha$  to examine the effect of  $\rho$  in the solution of (8.7.3), subject to the following initial condition:

$$u(x, 0) = \exp(-20(x)^2) + \frac{5}{2} \exp(-10(x - 4)^2) + 3 \exp(-20(x + 4)^2). \tag{8.7.15}$$

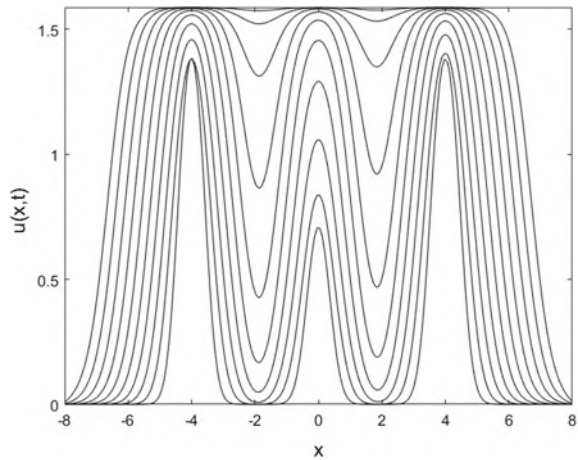
Other parameters are given as  $D = 0.38$ ,  $\kappa = 1$ ,  $L = 10$  with fractional power  $\alpha$  fixed at 0.91, and simulation time  $t = 1.5$ .

Next, we present the two-dimensional experiment for fractional Eq. (8.7.5) using the Caputo, Caputo–Fabrizio and Atangana–Baleanu fractional derivative operators.

**Fig. 8.3** 1D contour plot (8.7.3) when  $\alpha = 0.25$  and  $t = 1.0$  for  $L = 1$



**Fig. 8.4** 1D contour plot (8.7.3) when  $\alpha = 0.50$ ,  $L = 8$  and  $t = 1.0$

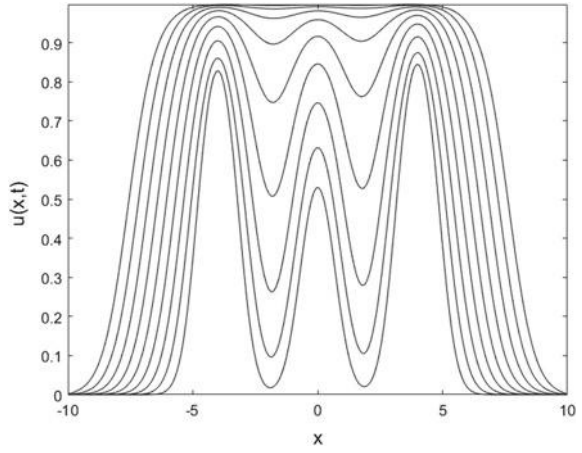


We first apply the Caputo derivative in Figs. 8.18, 8.19 and 8.20 using the initial condition

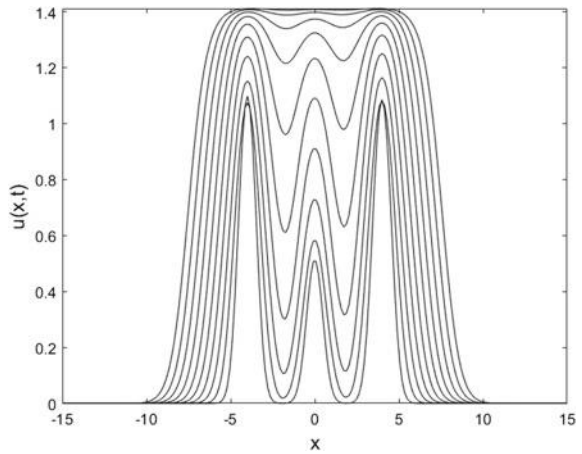
$$u_0(x, y) = \left[ \frac{1}{2} \tanh \left[ -\frac{\mu}{2\sqrt{2\mu+4}} \left( x - \frac{\mu+4}{2\sqrt{2\alpha+4}} y \right) \right] + \frac{1}{2} \right]^{2/\mu}, \quad (8.7.16)$$

where  $\mu \in [0.5, 1]$ .

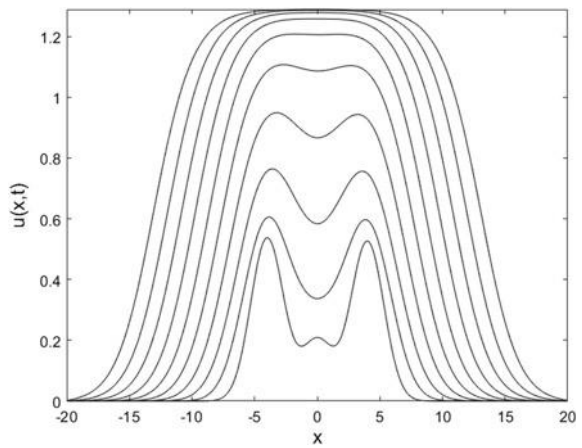
**Fig. 8.5** 1D contour plot (8.7.3) when  $\alpha = 0.55, L = 10$  and  $t = 1.0$



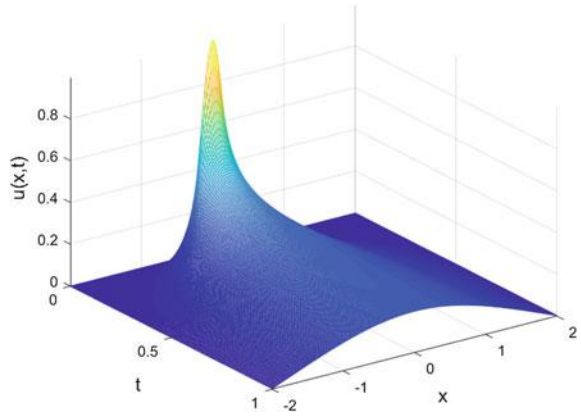
**Fig. 8.6** 1D contour plot (8.7.3) when  $\alpha = 0.59, L = 15$  and  $t = 1.0$



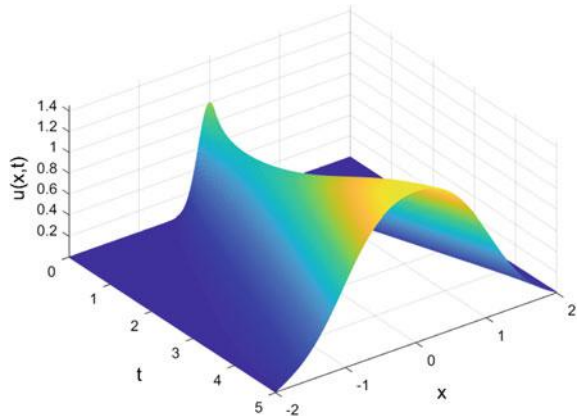
**Fig. 8.7** 1D contour plot (8.7.3) when  $\alpha = 0.62, L = 20$  and  $t = 1.0$



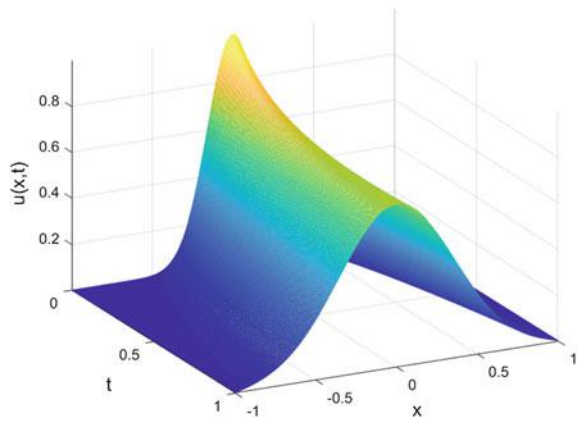
**Fig. 8.8** 1D surface plot for (8.7.3), with  $\alpha = 0.48$



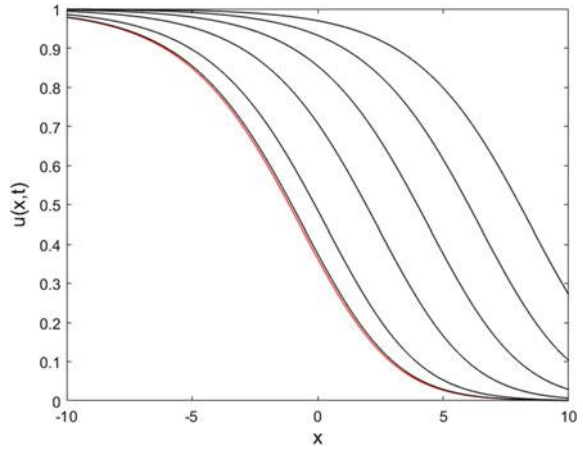
**Fig. 8.9** 1D surface plot for (8.7.3), with  $\alpha = 0.57$



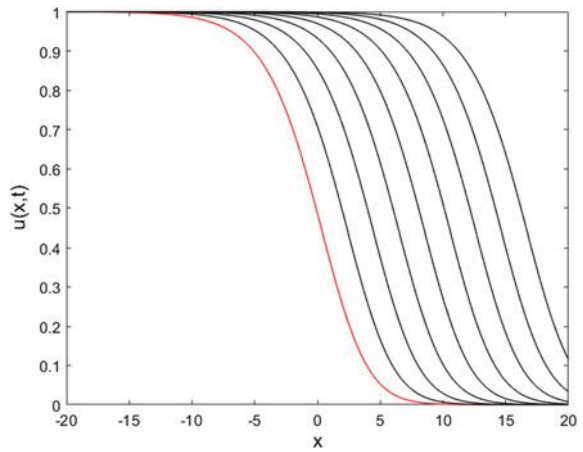
**Fig. 8.10** 1D surface plot for (8.7.3), with  $\alpha = 0.63$



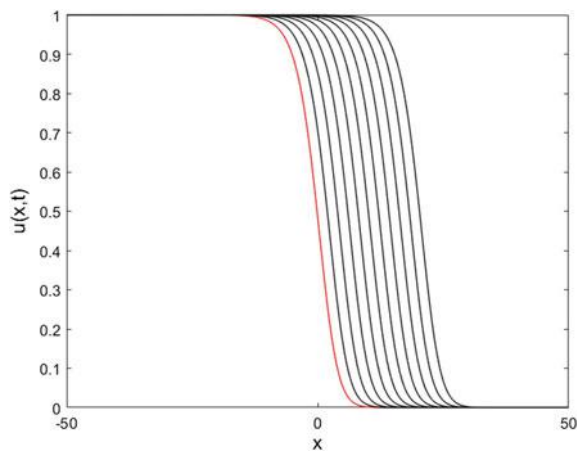
**Fig. 8.11** Numerical solution for (8.7.3), with  $L = 10$  and  $\alpha = 0.93$



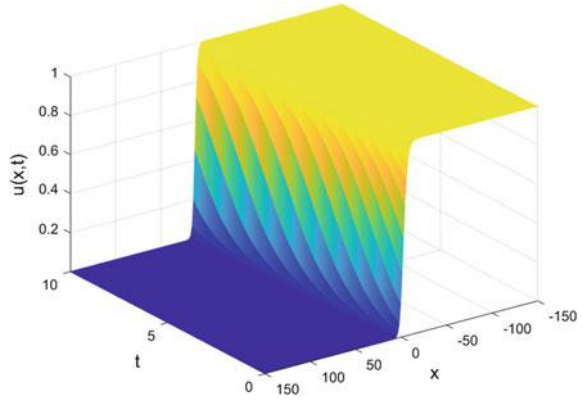
**Fig. 8.12** Numerical solution for (8.7.3), with  $L = 20$  and  $\alpha = 0.93$



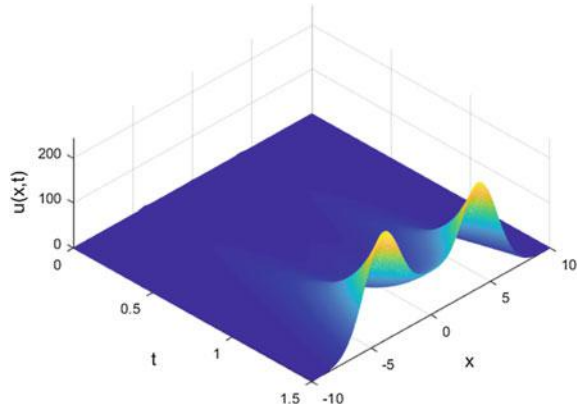
**Fig. 8.13** Numerical solution for (8.7.3), with  $L = 50$  and  $\alpha = 0.93$



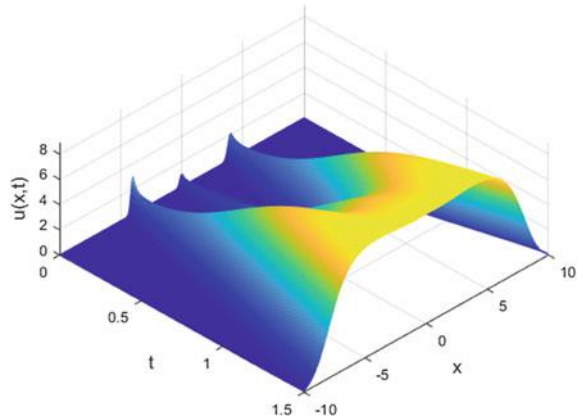
**Fig. 8.14** Surface plot for (8.7.3), with  $L = 150$  and  $\alpha = 0.89$



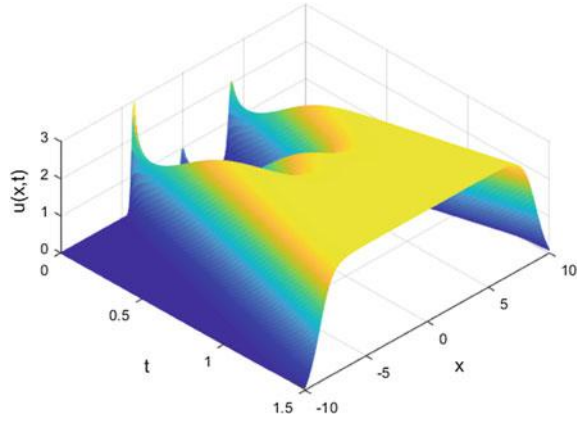
**Fig. 8.15** Solution of (8.7.3), with  $\rho = 1$  and  $\alpha = 0.91$



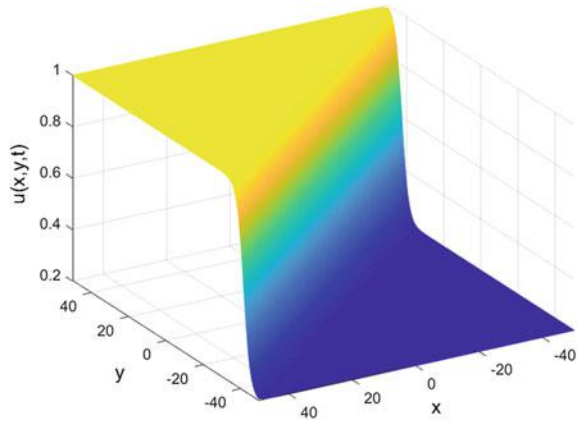
**Fig. 8.16** Solution of (8.7.3), with  $\rho = 2$  and  $\alpha = 0.91$



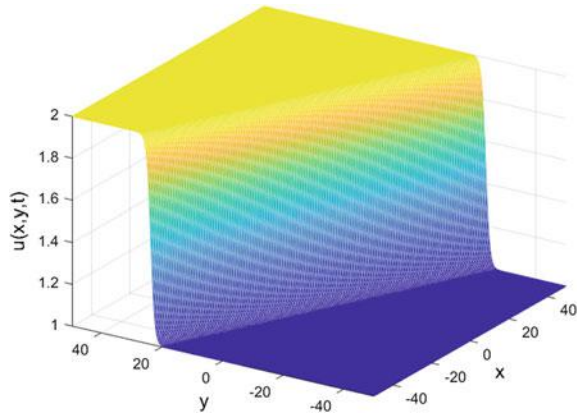
**Fig. 8.17** Solution of (8.7.3), with  $\rho = 3$  and  $\alpha = 0.91$



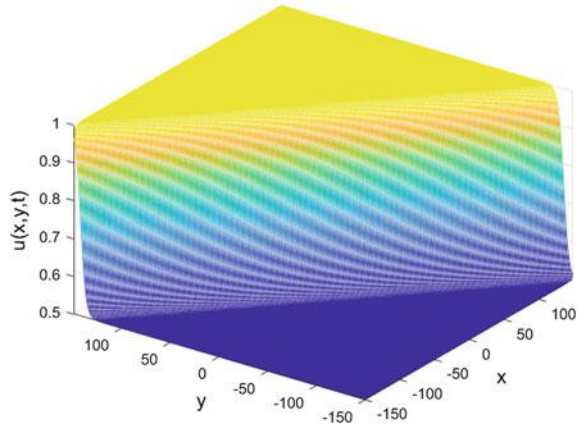
**Fig. 8.18** 2D result for (8.7.5) with  $\alpha = 0.87$



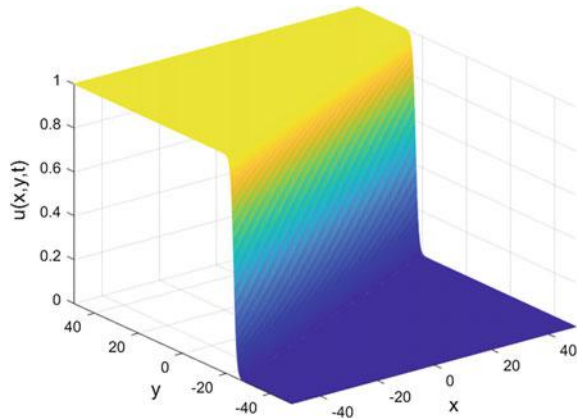
**Fig. 8.19** 2D result for (8.7.5) with  $\alpha = 0.89$



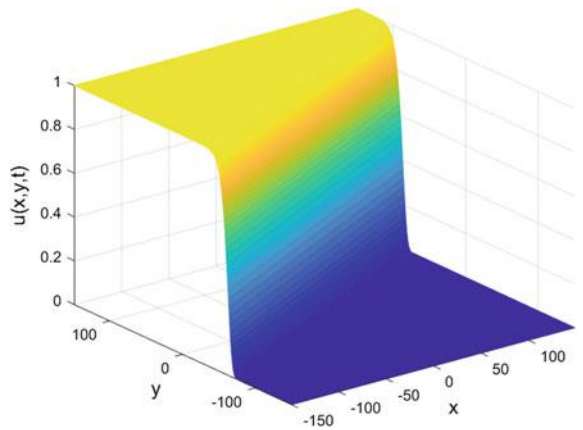
**Fig. 8.20** 2D result for (8.7.5) with  $\alpha = 0.95$



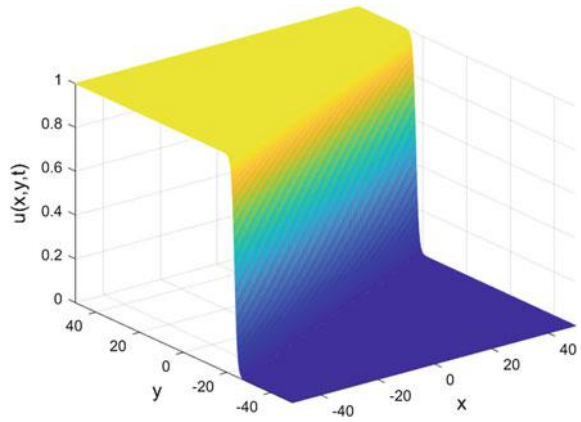
**Fig. 8.21** 2D result for (8.7.5) with  $\alpha = 0.73$



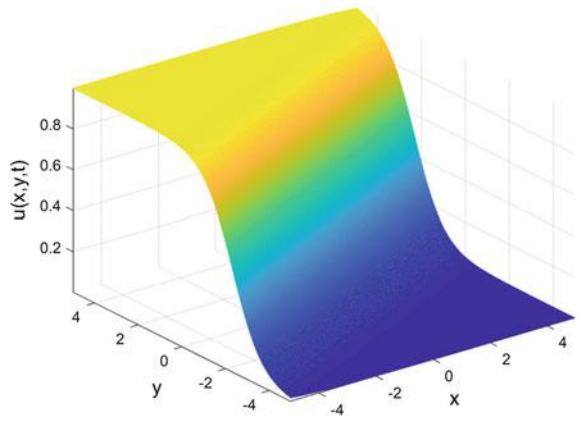
**Fig. 8.22** 2D result for (8.7.5) with  $\alpha = 0.79$



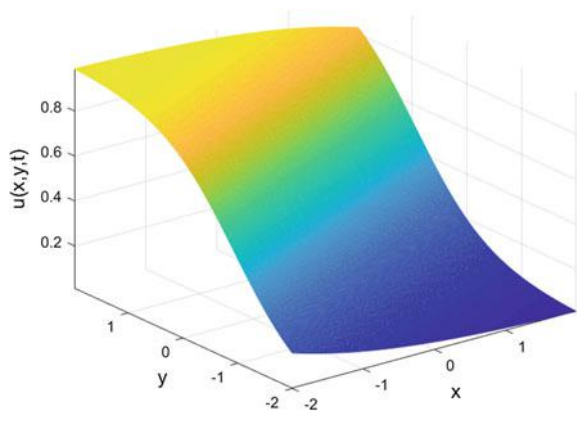
**Fig. 8.23** 2D result for (8.7.5) with  $\alpha = 0.83$



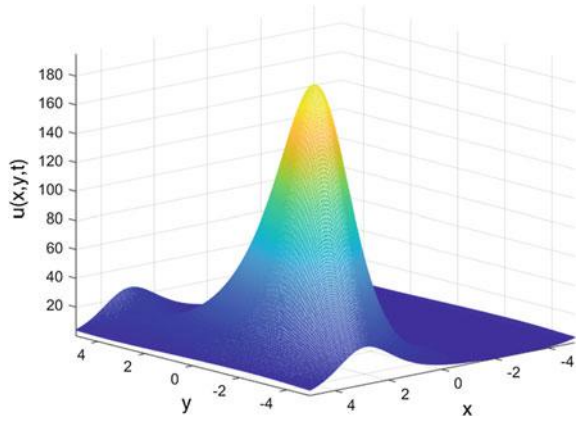
**Fig. 8.24** 2D result for (8.7.5) with  $\alpha = 0.88$



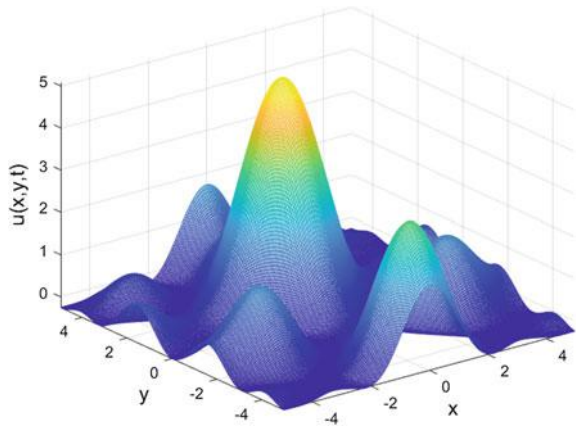
**Fig. 8.25** 2D result for (8.7.5) with  $\alpha = 0.91$



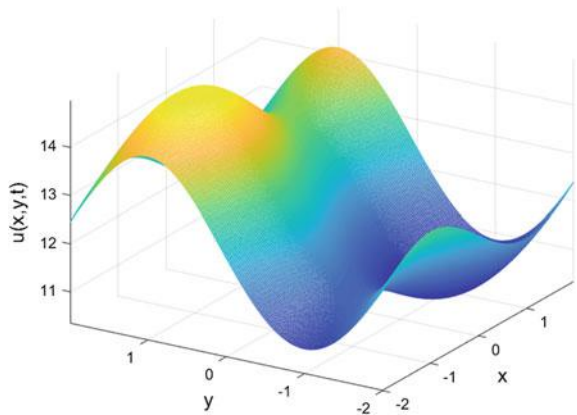
**Fig. 8.26** 2D result for (8.7.5) with  $\alpha = 0.55$

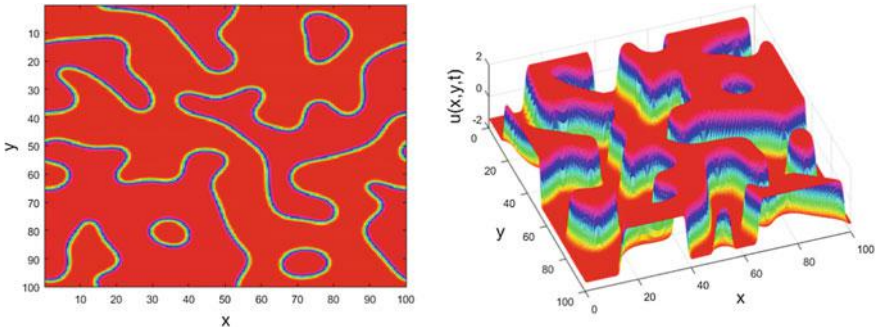


**Fig. 8.27** 2D result for (8.7.5) with  $\alpha = 0.41$

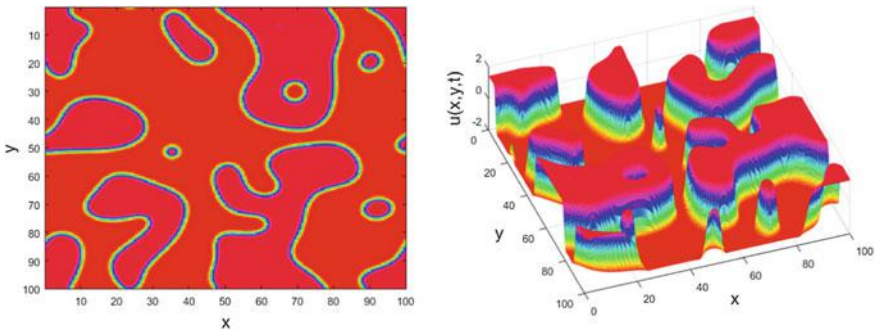


**Fig. 8.28** 2D result for (8.7.5) with  $\alpha = 0.94$

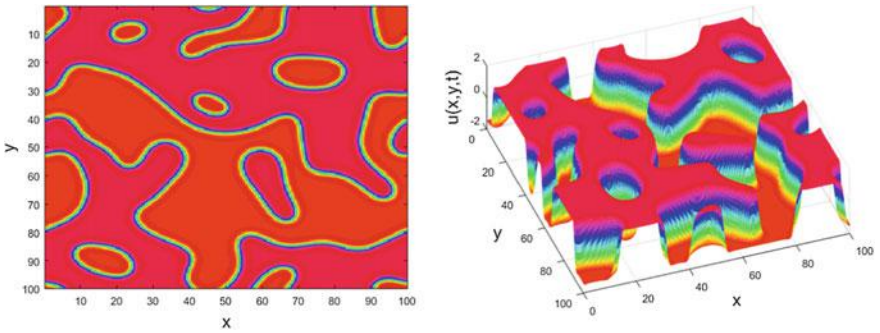




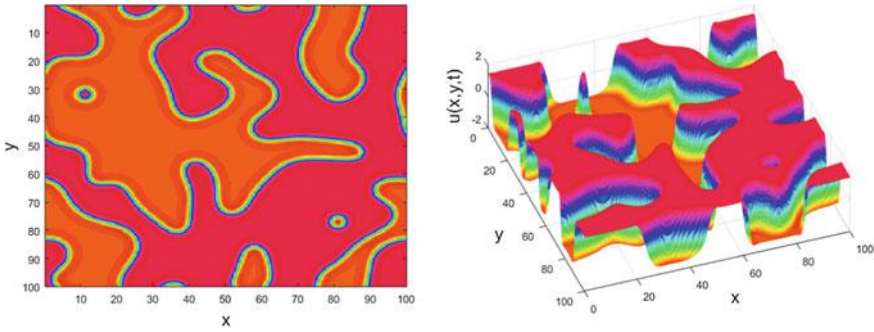
**Fig. 8.29** 2D snapshot and surface plot result for (8.7.5) with  $\alpha = 0.25$



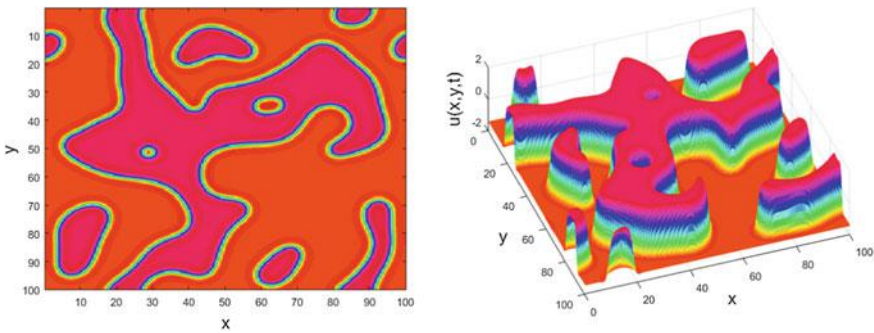
**Fig. 8.30** 2D snapshot and surface plot result for (8.7.5) with  $\alpha = 0.41$



**Fig. 8.31** 2D snapshot and surface plot result for (8.7.5) with  $\alpha = 0.74$



**Fig. 8.32** 2D snapshot and surface plot result for (8.7.5) with  $\alpha = 0.86$

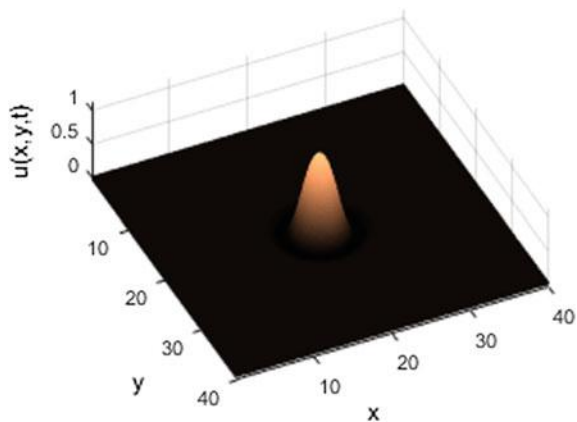


**Fig. 8.33** 2D snapshot and surface plot result for (8.7.5) with  $\alpha = 0.98$

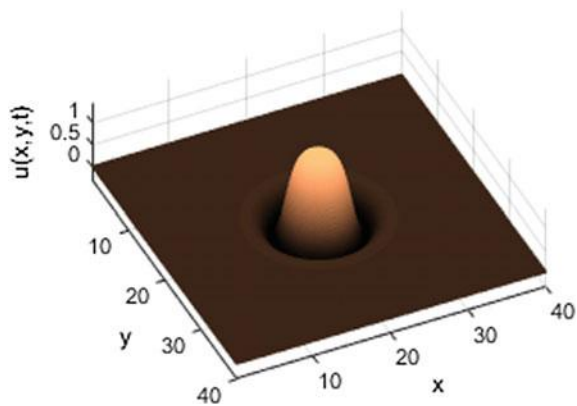
Second, we apply the Caputo–Fabrizio operator to Eq. (8.7.5) to obtain Figs. 8.21, 8.22, 8.23, 8.24 and 8.25. Lastly, we use the Atangana–Baleanu derivative to obtain Figs. 8.26, 8.27 and 8.28.

The next 2D experiment applies the Atangana–Baleanu derivative of order  $\alpha$ , subject to the zero-flux boundary condition mounted at the extreme ends of the domain  $x \in [-L, L]$  and the initial condition  $u(x, y, t = 0)$  obtained from a random normal distribution of about 0.55. The simulation results obtained for different instances of  $\alpha$  are displayed in Figs. 8.29, 8.30, 8.31, 8.32 and 8.33 captions. Other parameters given as  $D = 0.15$ ,  $\beta = 0.50$ ,  $\kappa = 2$ ,  $\rho = 2$  and  $L = 100$ . This type of model has a lot of applications in fractals and groundwater studies. Simulation runs for  $t = 150$ . Further, we verified the effect of varying the simulation time  $t$  for  $\alpha = 0.66$  in Figs. 8.34, 8.35, 8.36 and 8.37. In Figs. 8.38, 8.39, 8.40 and 8.41, we simulate with  $t = 150$  for different instances of  $\alpha$  as shown in the captions.

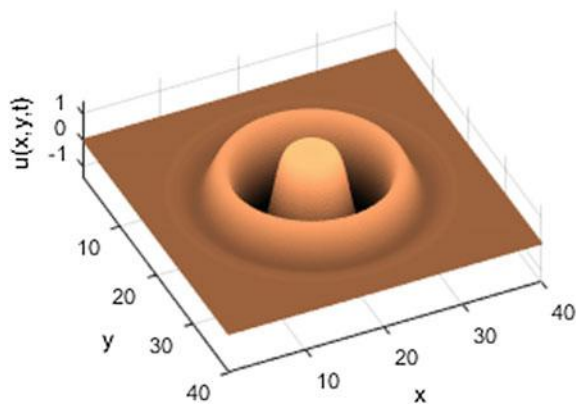
**Fig. 8.34** 2D surface plot for (8.7.5) at  $t = 5$



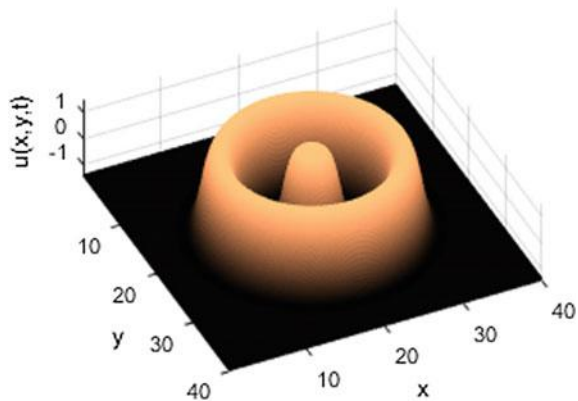
**Fig. 8.35** 2D surface plot for (8.7.5) at  $t = 10$



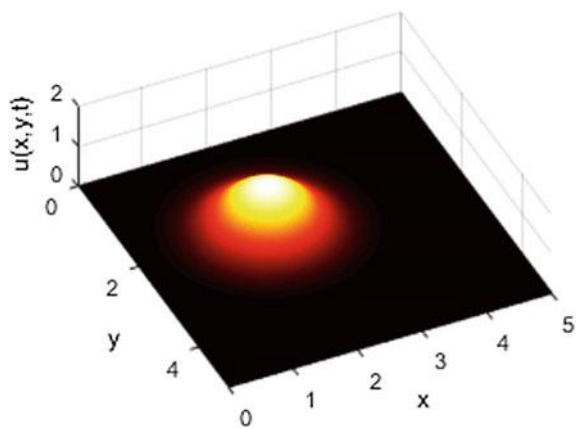
**Fig. 8.36** 2D surface plot for (8.7.5) at  $t = 20$



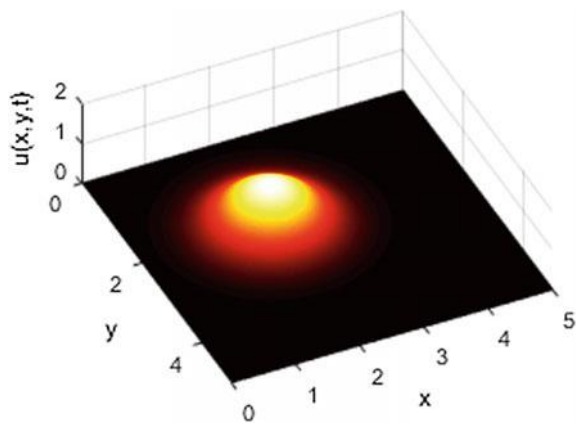
**Fig. 8.37** 2D surface plot  
for (8.7.5) at  $t = 50$



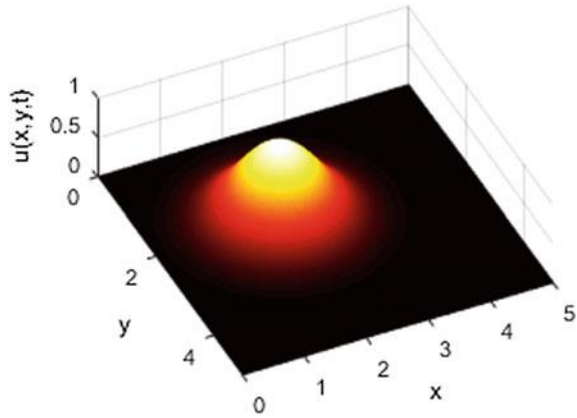
**Fig. 8.38** 2D surface plot  
for (8.7.5) at  $\alpha = 0.25$



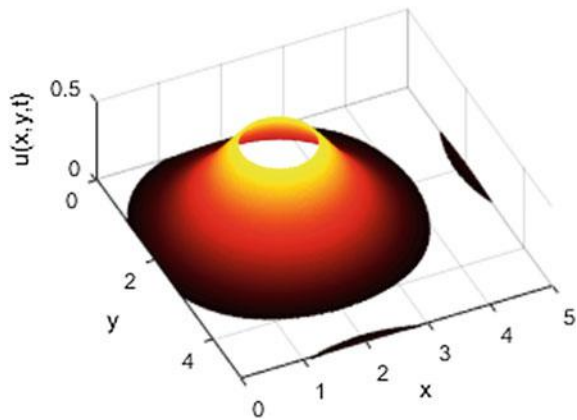
**Fig. 8.39** 2D surface plot  
for (8.7.5) at  $\alpha = 0.50$



**Fig. 8.40** 2D surface plot for (8.7.5) at  $\alpha = 0.75$



**Fig. 8.41** 2D surface plot for (8.7.5) at  $\alpha = 0.93$



### 8.7.2 The Gray–Scott Model

The Gray–Scott system was formulated by P. Gray and S.K. Scott at the University of Leeds in the early 1980s [21, 22]. Gray and Scott started with the isothermal autocatalytic equations in the continuously flowing well-stirred tank reactor (CSTR). In the model, isothermal means the reaction takes place at constant temperature, autocatalytic implies that the catalyst is also the product and continuously flowing corresponds to an open system. The well-stirred assumption indicates a system involving uniform transport of reactants.

The derivation of Gray–Scott system corresponds to the following two irreversible chemical reactions [21, 51, 66]:



where  $P$  is an inert product. The above system shows that one unit of agent  $U$  reacts with two units of  $V$  to form three units of  $V$ . By denoting the concentrations of the chemicals  $U$  and  $V$  by  $u$ ,  $v$ , the resulting reaction–diffusion system in dimensionless units becomes

$$\begin{aligned}\frac{\partial u}{\partial t} &= D_u \Delta^2 u - uv^2 + F(1 - u) \\ \frac{\partial v}{\partial t} &= D_v \Delta^2 v + uv^2 - v(F + k),\end{aligned}\tag{8.7.19}$$

where  $k$  and  $F$  are the dimensionless rate constant and feed rate, respectively.  $D_u$  and  $D_v$  are dimensionless diffusion coefficients of the respective chemical species  $U$  and  $V$ . A lot of research work based on (8.7.19) has been conducted, among which are the numerical solution of singular patterns in one- and two-dimensional Gray–Scott equations [56, 62], pulse splitting in 1D [16] and self-replicating structures [62, 70]. Also, in fractional form, Pindza and Owolabi considered the 2D simulation of space-fractional Gray–Scott model [67].

In this chapter, we are motivated with the formulation of time-fractional Gray–Scott model

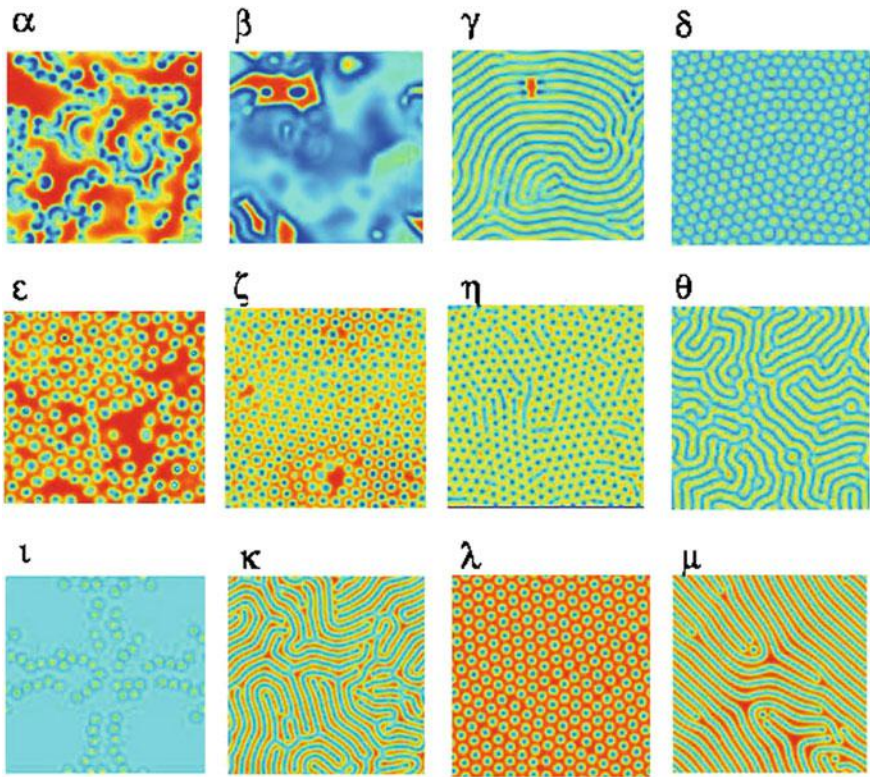
$$\begin{aligned}\mathcal{D}_t^\alpha u &= D_u \Delta^2 u - uv^2 + F(1 - u) \\ \mathcal{D}_t^\alpha v &= D_v \Delta^2 v + uv^2 - v(F + k),\end{aligned}\tag{8.7.20}$$

where  $\mathcal{D}_t^\alpha$  can be approximated by the Caputo, Caputo–Fabrizio or the Atangana–Baleanu fractional derivatives.

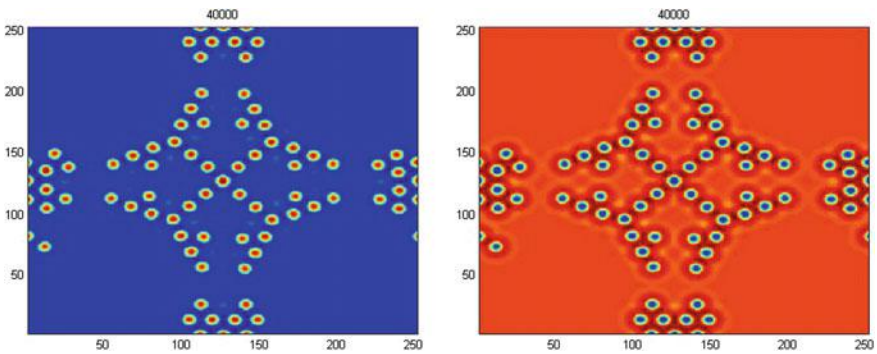
In the simulation framework, we set  $u = u(x, y, t)$  or  $u = u(x, y, z, t)$  with similar expressions for  $v$  in two and three dimensions. In 2D, we experiment (8.7.20) on a square domain size  $[0, 250] \times [0, 250]$  with no flux boundary conditions, the diffusion coefficients that represent the rate at which the chemical species diffuse in space are given as  $D_u = 2^{-5}$  and  $D_v = 10^{-5}$ . We assume  $x, y \in \mathbf{R}^2$ , and the Laplacian operator  $\Delta^2 = (\partial^2/\partial x^2 + \partial^2/\partial y^2)$ . We take  $\Delta x = 0.01$  and the time step  $\Delta t = 0.25$ . Simulation experiments in one dimension are omitted here.

Figure 8.42 shows the original patterns obtained by the Pearson for solution of classical Gray–Scott equations. The pure spots patterns in Figs. 8.43, 8.44 and 8.45 are obtained with  $F = 0.0208$  and  $k = 0.052$  for different values of  $\alpha$  at final simulation time  $t = 40000$ . The mixture of spots and stripes patterns as shown in Figs. 8.46, 8.47, 8.48, 8.49, 8.50 and 8.51 are obtained with  $F = 0.04$  and  $k = 0.06$  for different  $\alpha$  values.

Again, by setting  $F = 0.022, 0.042$  and  $k = 0.056, 0.066$ , one obtains different stripes structures for different values of fractional power  $\alpha$ . This assertion is evident in Figs. 8.52, 8.53, 8.54, 8.55, 8.56 and 8.57. Apart from the patterns obtaining Pearson, a range of mitotic and chaotic structures were obtained, see Figs. 8.58, 8.59 and 8.60 for chaotic patterns at  $F = 0.02$  and  $k = 0.05$ . Setting  $F = 0.028$  and  $k = 0.054$  for different values of  $\alpha$  gives rise to what is called mitotic-spots-like patterns as

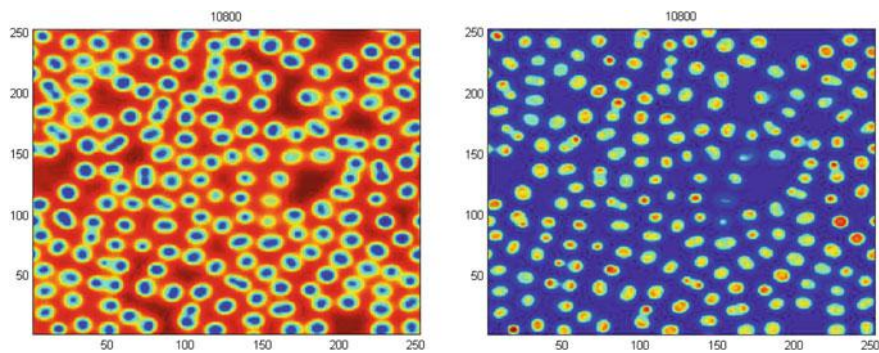


**Fig. 8.42** Classical 2D results obtained by Pearson [66] for different values of  $F$  and  $A$

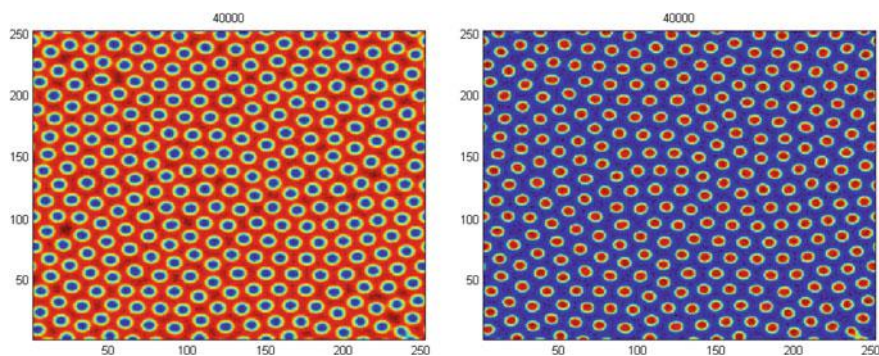


**Fig. 8.43** Formation of spots pattern for  $\alpha = 0.25$

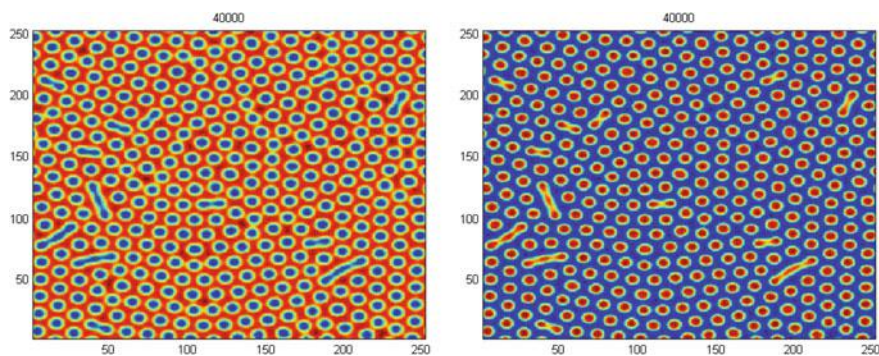
shown in Figs. 8.61 and 8.62. Finally, with  $F = 0.045$  and  $k = 0.06$ , we obtained a spatiotemporal spiral-like patterns for  $\alpha = 0.12$  and  $\alpha = 0.70$ , as shown in Figs. 8.63 and 8.64, respectively.



**Fig. 8.44** Formation of spots pattern for  $\alpha = 0.53$



**Fig. 8.45** Formation of spots pattern for  $\alpha = 0.93$



**Fig. 8.46** Mixture of spots and stripe structures for  $\alpha = 0.15$

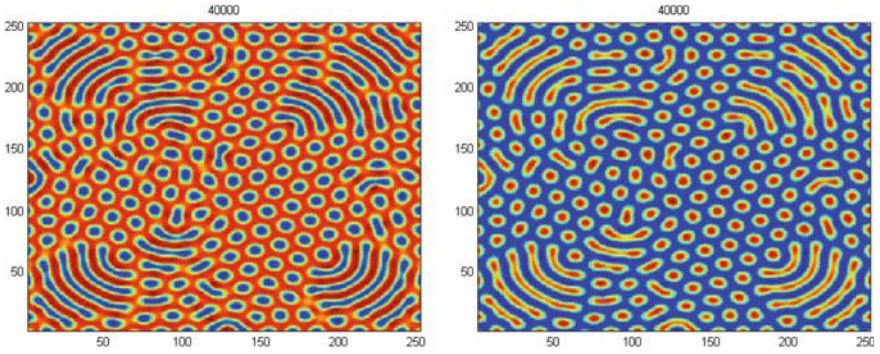


Fig. 8.47 Mixture of spots and stripe structures for  $\alpha = 0.23$

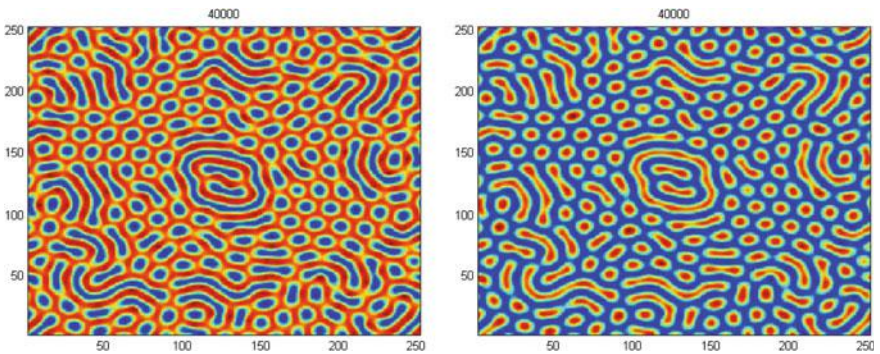


Fig. 8.48 Mixture of spots and stripe structures for  $\alpha = 0.41$

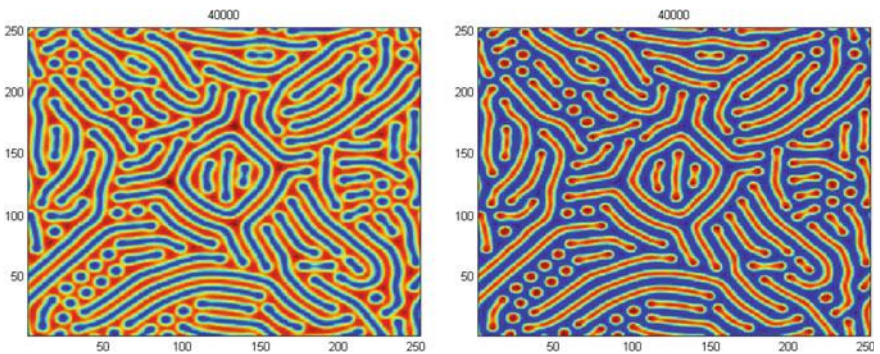


Fig. 8.49 Mixture of spots and stripe structures for  $\alpha = 0.68$

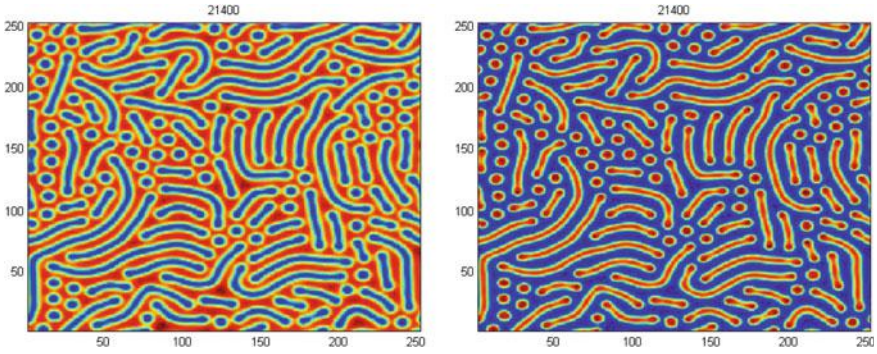


Fig. 8.50 Mixture of spots and stripe structures for  $\alpha = 0.79$

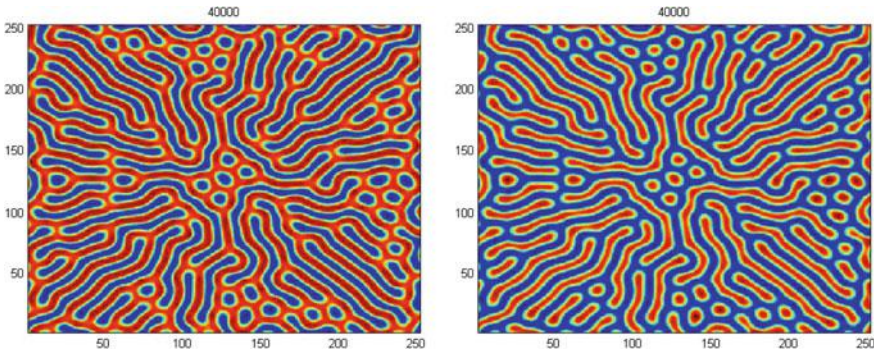


Fig. 8.51 Mixture of spots and stripe structures for  $\alpha = 0.91$

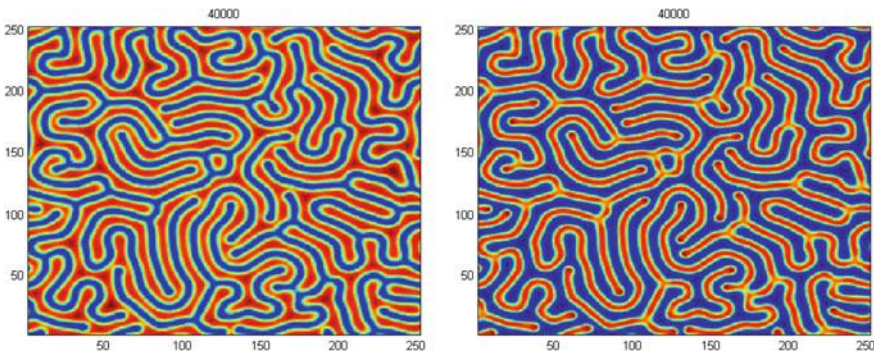
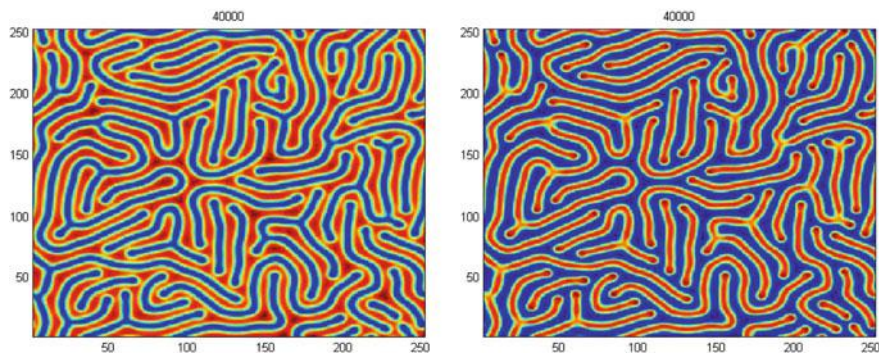
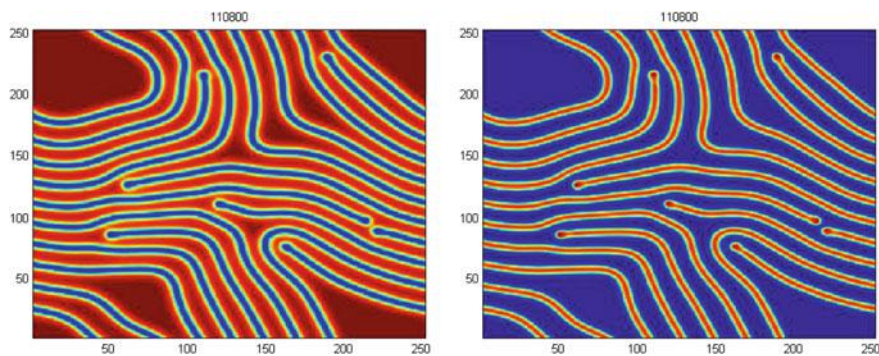


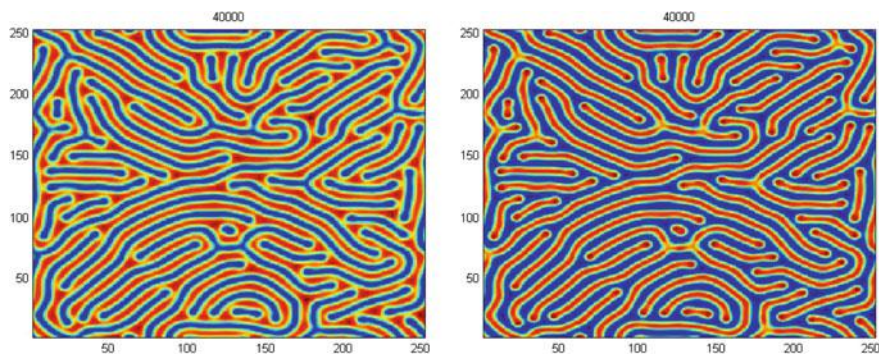
Fig. 8.52 Formation of pure stripe pattern for  $\alpha = 0.59$



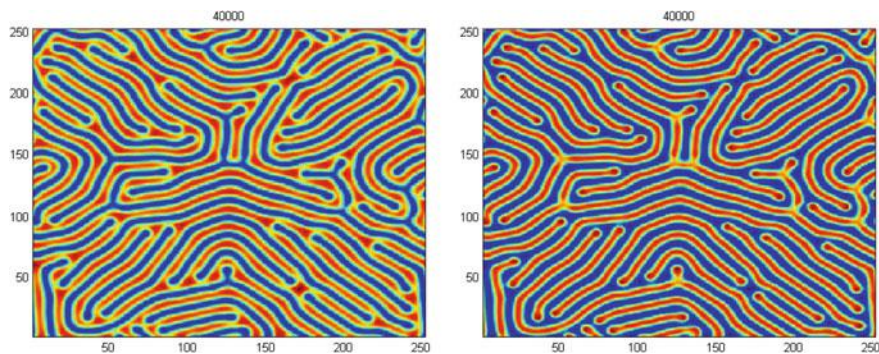
**Fig. 8.53** Formation of pure stripe pattern for  $\alpha = 0.69$



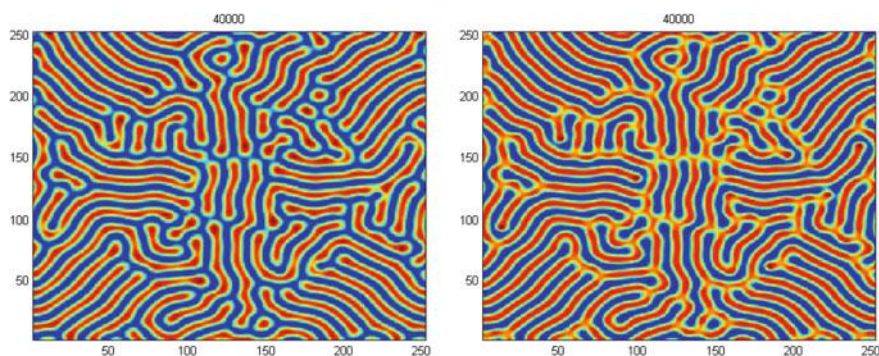
**Fig. 8.54** Formation of pure stripe pattern for  $\alpha = 0.23$



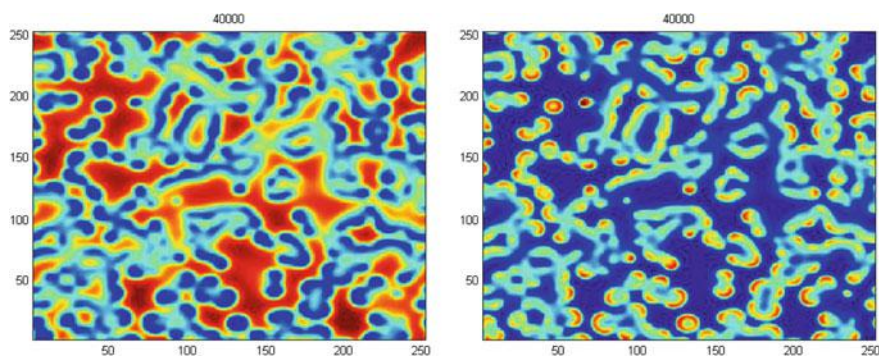
**Fig. 8.55** Formation of pure stripe pattern for  $\alpha = 0.77$



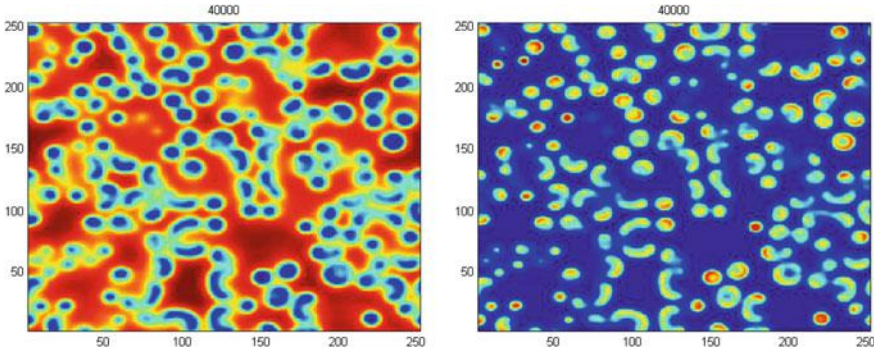
**Fig. 8.56** Formation of pure stripe pattern for  $\alpha = 0.80$



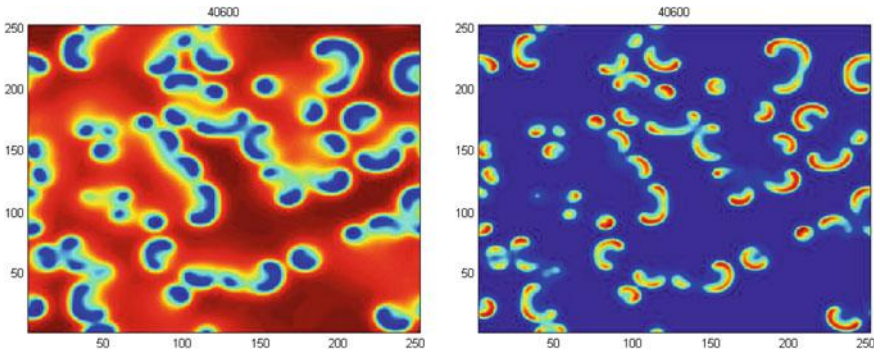
**Fig. 8.57** Formation of pure stripe pattern for  $\alpha = 0.85$



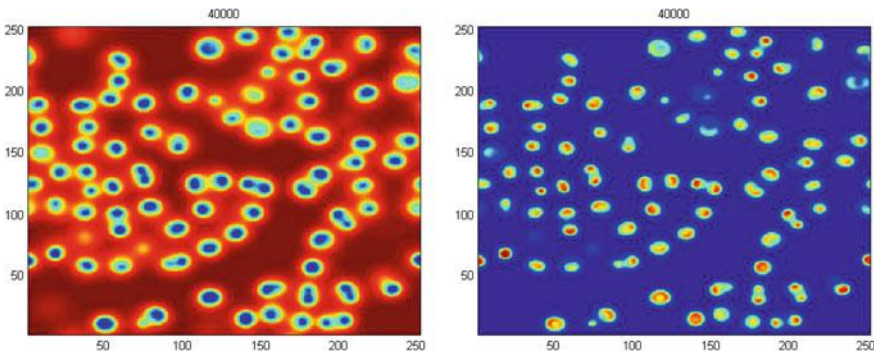
**Fig. 8.58** Chaotic pattern for  $\alpha = 0.38$



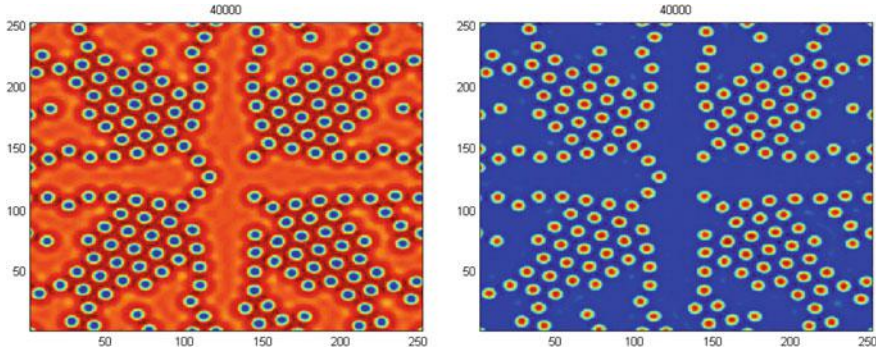
**Fig. 8.59** Chaotic pattern for  $\alpha = 0.45$



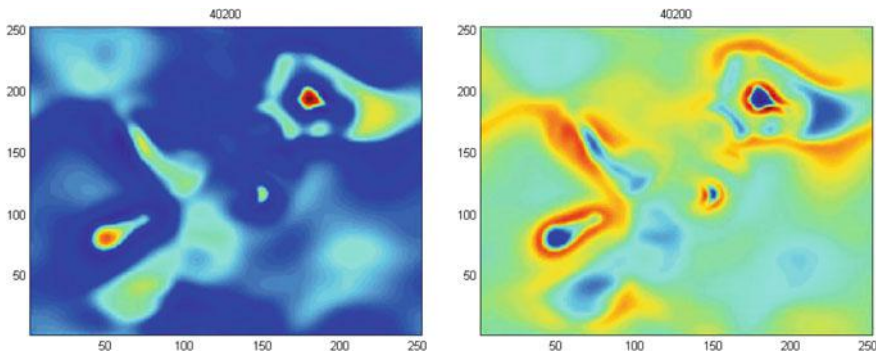
**Fig. 8.60** Chaotic pattern for  $\alpha = 0.55$



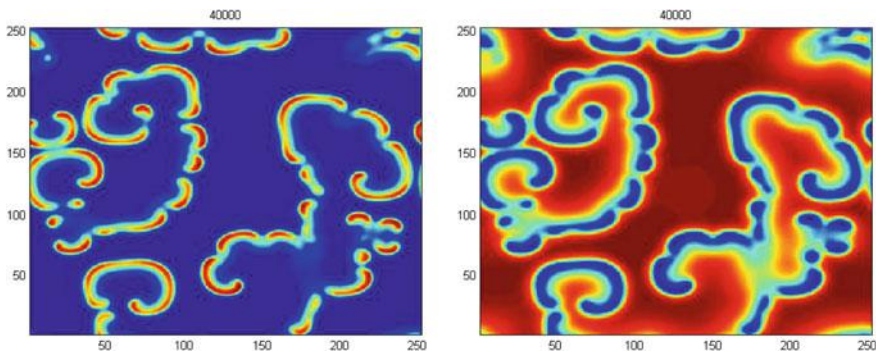
**Fig. 8.61** Mitotic pattern for  $\alpha = 0.42$



**Fig. 8.62** Mitotic pattern for  $\alpha = 0.93$



**Fig. 8.63** Spatiotemporal spiral-like pattern for  $\alpha = 0.12$



**Fig. 8.64** Spatiotemporal spiral-like pattern for  $\alpha = 0.70$

Clearly, modelling with fractional derivatives could result in the emergence of brand new structures that are not likely to be found in the classical models. It should be mentioned that the distribution of species  $u$  and  $v$  is almost similar, for the sake of

clarity, we reported both here. Also, apart from the patterns reported in this chapter, other known structures can be obtained depending on the choices of initial data and other parameters.

Next, we experiment the dynamic richness of time-fractional Gray–Scott model (8.7.20) in three spatial dimensions, that is,

$$\begin{aligned} {}_0^C \mathcal{D}_t^\alpha &= D_u \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) + F(1 - u) \\ {}_0^C \mathcal{D}_t^\alpha &= D_v \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) + uv^2 - v(F + k), \end{aligned} \quad (8.7.21)$$

where  $u = u(x, y, z)$  and  $v = v(x, y, z)$ . The term  ${}_0^C \mathcal{D}_t^\alpha$  is the usual Caputo fractional derivative of order  $\alpha$ . System (8.7.21) is numerically solved on large but finite domain size  $x, y, z \in [-L, L]$  subject to the zero-flux boundary conditions and initial functions [67]

$$\begin{aligned} u(x, y, z, 0) &= 1 - 0.5 \exp \left[ -50 \left( \left( x - \frac{\varphi}{2} \right)^2 + \left( y - \frac{\varphi}{2} \right)^2 + \left( z - \frac{\varphi}{2} \right)^2 \right) \right], \\ v(x, y, z, 0) &= 0.25 \exp \left[ -50 \left( \left( x - \frac{\varphi}{2} \right)^2 + 2 \left( y - \frac{\varphi}{2} \right)^2 + \left( z - \frac{\varphi}{2} \right)^2 \right) \right]. \end{aligned} \quad (8.7.22)$$

## 8.8 Application of Riesz Fractional Derivative to Schrödinger Equation

The classical Schrödinger equation is considered as a basic equation used in applied area of quantum mechanics for studying the evolution and dynamics of wave packets over the last few decades. Some years ago, the classical Schrödinger equation has been generalized to a fractional partial differential equation (FPDE) where the Riesz space-fractional derivative is used as against the conventional Laplacian operator [37, 60]. Zhang et al. [80] examined the propagation of waves in noninteger-order Schrödinger equation with harmonic potential, as well as uniform acceleration [68]. Also, the case  $\alpha = 1$  has been considered by Liemert and Kienle [39] for studying the propagation of the wave packets that undergo splitting and spreading.

A few possibilities of numerical implementations of fractional-order derivatives can be found in [12, 14, 67]. Here, we consider the following time-dependent fractional nonlinear Schrödinger equation with the Riesz fractional-in-space derivative of order  $0 < \alpha \leq 2$  [3, 37, 60]

$$\left. \begin{aligned} i \frac{\partial u(\mathbf{x}, t)}{\partial t} &= \frac{1}{2} (-\Delta)^{\alpha/2} u(\mathbf{x}, t) + P(\mathbf{x}) u(\mathbf{x}, t) + \beta |u(\mathbf{x}, t)|^2 u(\mathbf{x}, t) \\ u(\mathbf{x}, 0) &= u_0(\mathbf{x}), \quad \mathbf{x} \in \mathbf{R}, \end{aligned} \right\} \quad (8.8.1)$$

where  $(\mathbf{x}, t)$  represents the complex-valued wave function for vector  $\mathbf{x} \in \mathbf{R}$  and time  $t > 0$ ,  $\beta \in \mathbf{R}$  denotes the strength of local interactions. The real-valued function  $P(x)$  is an external trapping (harmonic) potential written in the form

$$V(\mathbf{x}) = \frac{1}{2} \begin{cases} \gamma_x^2 x^2, \\ \gamma_x^2 x^2 + \gamma_y^2 y^2, \\ \gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2, \end{cases} \quad \mathbf{x} \in \mathbf{R}, \quad (8.8.2)$$

where  $\gamma_x$ ,  $\gamma_y$  and  $\gamma_z$  are the dimensionless trapping frequencies in the spatial directions  $x$ ,  $y$  and  $z$ , respectively.

### 8.8.1 One-Dimensional Fractional-in-Space Schrödinger Equation

We demonstrate in one dimension (1D), the numerical illustration Schrödinger equation with linear potential  $P(x) = \gamma(x)$  is given by

$$i \frac{\partial u(x, t)}{\partial t} = \frac{1}{2} (-\Delta)^{\frac{\alpha}{2}} u(x, t) + \gamma(x) u(x, t), \quad x \in \mathbf{R}, \quad t > 0 \quad (8.8.3)$$

where  $u(x, t)$  is referred to as the wave function, the order of the Riesz operator is bounded on  $0 < \alpha \leq 2$ . By following [40, 41, 60], we give the occurrence of the noninteger operator in (8.8.3) as

$$\mathcal{F} \left\{ (-\Delta)^{\frac{\alpha}{2}} f(x) \right\} (\omega) = |\omega|^\alpha F(\omega), \quad (8.8.4)$$

where  $F(\omega) = \int_{-\infty}^{\infty} f(x) \exp(i\omega x) dx$  is the Fourier transform of  $f(x)$ . The solution of Eq. (8.8.3) is sought subject to conditions

$$u(x, 0) = u_0(x), \quad \lim_{|x| \rightarrow \infty} u(x, t) = 0 \quad (8.8.5)$$

with  $u_0(x)$  being the initial wave normalized w.r.t.  $\int_{-\infty}^{\infty} |u_0(x)|^2 dx = 1$ . In momentum space, we present the corresponding equation as

$$\begin{aligned} i \frac{\partial u(\omega, t)}{\partial t} &= \frac{1}{2} |\omega|^\alpha u(\omega, t) + i\gamma \frac{\partial u(\omega, t)}{\partial \omega}, \quad \omega \in \mathbf{R}, \quad t > 0, \\ u(\omega, 0) &= u_0(\omega). \end{aligned} \quad (8.8.6)$$

Now, we introduce a function  $u(\omega, t) = e^{ik(\omega)} v(\omega + \gamma t)$  and use it in (8.8.6) to have

$$i\gamma e^{ik} v'(\omega + \gamma t) = \frac{1}{2} |\omega|^\alpha e^{ik} v(\omega + \gamma t) + i\gamma e^{ik} v'(\omega + \gamma t) - \gamma e^{ik} v(\omega + \gamma t) \frac{dk}{d\omega},$$

where  $k, v$  are unknown and  $v'$  represents the first derivative of  $v$ . We compare both sides to obtain

$$\frac{dk(\omega)}{d\omega} = \frac{|\omega|^\alpha}{2\gamma}$$

which can be addressed directly by using the function

$$k(\omega) = \frac{\omega|\omega|^\alpha}{2\gamma(1+\alpha)} + a, \quad (a \text{ is an arbitrary constant}), \quad \omega \in \mathbf{R}.$$

By using the initial condition, we obtain the  $v$  according to

$$u(\omega, 0) = u_0(\omega) = e^{ik(\omega)}v(\omega) \Rightarrow v(\omega) = u_0(\omega)e^{-ik(\omega)}.$$

Thus, in momentum space the complete solution to (8.8.6) is

$$u(\omega, t) = u_0(\omega + \gamma t) \exp \left[ i \frac{\omega|\omega|^\alpha - (\omega + \gamma t)|\omega + \gamma t|^\alpha}{2\gamma(\alpha + 1)} \right], \quad \forall 0 < \alpha \leq 2. \quad (8.8.7)$$

In real space, the wave function is written in the form [2, 39, 42, 60]

$$u(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} u(x, t) e^{i\omega x} d\omega.$$

In terms of the convolution for the classical case of  $\alpha = 2$ , the wave function is written as

$$u(x, t) = \frac{e^{-i\gamma x t} e^{-i\gamma^2 t^3/6}}{\sqrt{2\pi i t}} \int_{-\infty}^{\infty} u_0(y) \exp \left[ i \frac{(x - y + \gamma t^2/2)^2}{2t} \right] dy.$$

The case  $\gamma = 0$  corresponds to the free state, which means that the momentum space Eq. (8.8.6) is now reduced to

$$u(\omega, t) = u_0(\omega) \exp(-it|\omega|^\alpha/2), \quad 0 < \alpha \leq 2.$$

### 8.8.2 Two-Dimensional Fractional-in-Space Schrödinger Equation

Here, we give an extension to 1D case by reporting the two-dimensional (2D) fractional Schrödinger equation with potential  $P(\mathbf{s}) = \mathbf{F} \cdot \mathbf{s}$  by

$$i \frac{\partial u(\mathbf{s}, t)}{\partial t} = \frac{1}{2} (-\Delta)^{\frac{\alpha}{2}} u(\mathbf{s}, t) + V(\mathbf{s}) u(\mathbf{s}, t), \quad \mathbf{s} \in \mathbf{R}^2, \quad t > 0, \quad (8.8.8)$$

where  $\mathbf{F} = (F_1, F_2)$  and  $F = |\mathbf{F}|$ . Here, we define the 2D fractional Laplacian by

$$\mathcal{F}\{(-\Delta)^{\frac{\alpha}{2}} f(\mathbf{s})\}(\mathbf{r}) = |\mathbf{r}|^\alpha F(\mathbf{r}), \quad (8.8.9)$$

where  $|\mathbf{r}| = r$  denotes the length of the wave vector  $\mathbf{r} = (r_1, r_2)$  which has the Fourier transform  $F(\mathbf{r}) = \int f(\mathbf{s}) \exp(-i\mathbf{r} \cdot \mathbf{s}) d\mathbf{s}$ . Also, with  $\alpha = 1$ , we can formulate the 2D fractional Laplacian representation in the form

$$(-\Delta)^{\frac{1}{2}} f(\mathbf{s}) = \nabla \cdot R\{f(\mathbf{s})\}, \quad (8.8.10)$$

where  $R$  is the Riesz transform that maps the function  $f(\mathbf{s})$  into a vector field according to

$$R\{f(\mathbf{s})\} = \frac{1}{2\pi} \int \frac{f(\rho)(\mathbf{s} - \rho)}{|\mathbf{s} - \rho|} d\rho. \quad (8.8.11)$$

It should be mentioned that the relation (8.8.10) is the generalization of one-dimensional differential operator [42]

$$(-\Delta)^{\frac{1}{2}} f(x) = \mathcal{F}^{-1}\{|\omega|F(\omega)\}(x) = \frac{d}{dx} \mathcal{H}\{f(x)\},$$

where  $\mathcal{H}$  is the Hilbert transform defined by

$$\mathcal{H}\{f(x)\} = \frac{1}{\pi} \mathcal{P} \int_{-\infty}^{\infty} \frac{f(y)}{x - y} dy$$

and  $\mathcal{P}$  is the Cauchy principal value.

In 2D, the initial-boundary condition takes the form

$$u(\mathbf{s}, 0) = u_0(\mathbf{s}), \quad \lim_{s \rightarrow \infty} u(\mathbf{s}, t) = 0, \quad (8.8.12)$$

where  $\mathbf{s} = |\mathbf{s}|$ . In momentum space, Eq. (8.8.8) gives

$$\frac{\partial u(\mathbf{r}, t)}{\partial t} = \frac{r^\alpha}{2i} u(\mathbf{r}, t) + \mathbf{F}u(\mathbf{r}, t), \quad \mathbf{r} \in \mathbf{R}^2, \quad t > 0. \quad (8.8.13)$$

Similar to case 1D, one can seek a wave function in the form  $u(\mathbf{r}, t) = \exp[iv(\mathbf{r})] \varphi(\mathbf{r} + \mathbf{F}t)$ . By inserting this ansatz into (8.8.13), it results in the partial differential equation (PDE)

$$F_1 \frac{\partial v(\mathbf{r})}{\partial r_1} + F_2 \frac{\partial v(\mathbf{r})}{\partial r_2} = \frac{r^\alpha}{2}.$$

We realized the difficulty involves in solving fractional differential equation of order  $\alpha$ . But for the case  $\alpha = 1$ , the exact solution is formulated as

$$v(\mathbf{r}) = \frac{r}{4} \frac{F_1 r_1 + F_2 r_2}{F_1^2 + F_2^2} + \frac{1}{4} \frac{(F_1 r_2 + F_2 r_1)^2}{(F_1^2 + F_2^2)^{3/2}} \ln \left( 2r + 2 \frac{F_1 r_1 + F_2 r_2}{\sqrt{F_1^2 + F_2^2}} \right).$$

The classical case with  $\alpha = 2$  is not a problem to solve, we obtain the solution as

$$v(\mathbf{r}) = \frac{r_1^3}{3F_1} + \frac{r_2^3}{3F_2}.$$

Also, one can recover the unknown function  $\varphi$  with the initial condition

$$u(\mathbf{r}, 0) = u_0(\mathbf{r}) = \exp[iv(\mathbf{r})]\varphi(\mathbf{r}) \Rightarrow \varphi(\mathbf{r}) = u_0(\mathbf{r}) \exp[-iv(\mathbf{r})]. \quad (8.8.14)$$

For the wave function in momentum space, we obtain

$$u(\mathbf{r}, t) = u_0(\mathbf{r} + \mathbf{F}t) \exp[i(v(\mathbf{r}) - v(\mathbf{r} + \mathbf{F}t))]$$

and for the free particle type with  $\mathbf{F} = 0$ , the momentum space solution for all fractional orders is given as

$$u(\mathbf{r}, t) = u_0(\mathbf{r}) \exp\left(-\frac{itr^\alpha}{2}\right), \quad 0 < \alpha \leq 2.$$

### 8.8.3 Numerical Methods of Discretization

A lot of numerical approximation techniques have been introduced for the solution of a range of fractional reaction–diffusion problems [12, 24, 25, 28, 78, 79, 81]. Solving the linear system of the form  $\mathbf{A}\mathbf{u} = \mathbf{b}$  is computationally involving due to non-local nature of the fractional Laplacian operator  $(-\Delta)^{\alpha/2}$  which results in a full matrix representation of the fractional operator [59, 60, 67]. For this case, we apply the Spectral method in conjunction with both the fourth-order exponential time-differencing Runge–Kutta scheme to solve the time-dependent fractional Schrödinger equation in one and higher dimensions.

In one dimension, we consider the non-local case of the Schrödinger equation

$$\begin{aligned} i \frac{\partial u(x, t)}{\partial t} &= \tau(-\Delta)^{\frac{\alpha}{2}} u + \gamma(x)u + \beta|u|^{2\delta}, \quad x \in \Omega, \quad t > 0 \\ u(x, 0) &= u_0(x), \quad x \in \Omega. \end{aligned} \quad (8.8.15)$$

Equation (8.8.3) corresponds to  $\tau = \frac{1}{2}$  and  $\delta = 1$  in (8.8.1). We choose a periodic boundary condition valid for a large bounded domain  $\Omega \in \mathbf{R}^d$  truncated at, say,  $\pm L$ . Also, we let  $k > 0$ , a time step with sequence  $t_n = nk$ ,  $n = 0, 1, \dots$ . In two splitting steps, we solve (8.8.15) from  $t = t_n$  to  $t = t_{n+1}$ , that is,

$$i\partial_t u(x, t) = \tau(-\Delta)^{\frac{\alpha}{2}} u(x, t), \quad x \in \Omega, \quad t \in [t_n, t_{n+1}], \quad (8.8.16)$$

$$i\partial_t u(x, t) = \gamma(x)u(x, t) + \beta|u|^{2\delta}, \quad x \in \Omega, \quad t \in [t_n, t_{n+1}]. \quad (8.8.17)$$

Multiplying Eq. (8.8.17) with  $\bar{u}$ , add the resulting system to its complex conjugate, we obtain  $\partial_t (|u(x, t)|^2) = 0$ , which means that  $|u(x, t)|$  is the time invariant on  $[t_n, t_{n+1}]$ . As a result, we can write (8.8.17) for  $t_n \leq t \leq t_{n+1}$  to make it linear in  $u(x, t)$  as

$$i\partial_t u(x, t) = [\gamma(x) + \beta|u(x, t_n)|^{2\delta}]u(x, t), \quad x \in \Omega,$$

which on integration in time gives the solution to (8.8.17) as

$$u(x, t) = u(x, t_n) \exp[-i(\gamma(x) + \beta|u(x, t_n)|^{2\delta})(t - t_n)], \quad x \in \Omega, \quad t \in [t_n, t_{n+1}].$$

Following [3, 12, 53], we define the Riesz fractional laplacian  $(-\Delta)^{\frac{\alpha}{2}}$  by

$$(-\Delta)^{\frac{\alpha}{2}} u(x, t) := \mathcal{F}^{-1} [|\xi|^\alpha \mathcal{F} u], \quad x \in \mathbf{R}, \quad \alpha > 0, \quad t > 0, \quad (8.8.18)$$

where

$$\mathcal{F}(u)(\xi, t) = \int_{\mathbf{R}} u(x, t) e^{-i\xi \cdot x} dx, \quad \xi \in \mathbf{R}, \quad t > 0$$

is the Fourier transform  $u(x, t)$ , and its corresponding inverse is denoted by  $\mathcal{F}^{-1}$ . In fact, Eq. (8.8.18) is regarded as the pseudo-differential operator of the Riesz derivative  $(-\Delta)^{\frac{\alpha}{2}}$ . Due to definition in (8.8.18) and the periodic conditions in (8.8.15), for simplicity, we discretize (8.8.16) in just 1D, generalization to higher dimensions is quite simple and straightforward. Assume  $\omega \in [a, b]$ , we let the mesh  $h_x = (b - a)/N$ , for  $N > 0$ , and consider the grid points  $x_j = a + jh_x$ ,  $0 \leq j \leq N$ . We assume that

$$u(x, t) = \sum_{l=-N/2}^{N/2-1} \widehat{u}_l(t) \exp[i\nu_l(x - a)], \quad (8.8.19)$$

where  $\widehat{u}_l(t)$  stands for the Fourier transform of  $u(x, t)$  for frequency  $l$ , and

$$\nu_l = \frac{2l\pi}{b - a}, \quad -\frac{N}{2} \leq l \leq \frac{N}{2} - 1.$$

By putting (8.8.19) into (8.8.16), we get

$$i \frac{d\widehat{u}_l(t)}{dt} = \tau |\nu_l|^\alpha \widehat{u}_l(t), \quad -\frac{N}{2} \leq l \leq \frac{N}{2} - 1, \quad t_n \leq t \leq t_{n+1}. \quad (8.8.20)$$

Exact integration of (8.8.20) in time yields

$$\widehat{u}_l(t) = \widehat{u}_l(t_n) \exp[-i\tau|\nu_l|^\alpha(t - t_n)], \quad -\frac{N}{2} \leq l \leq \frac{N}{2} - 1, \quad t_n \leq t \leq t_{n+1}. \tag{8.8.21}$$

Note that the combination of (8.8.19) and (8.8.21) results in the solution of (8.8.16).

In this segment, we first apply the Strang splitting technique [74] to advance (8.8.15) and (8.8.16) from  $t = t_n$  to  $t = t_n + 1$ , we solve

$$u_j^{(1)} = u_j^{(n)} \exp \left\{ -i\frac{k}{2} [\gamma(x_j) + \beta|u_j^{(n)}|^{2\delta}] \right\},$$

$$u_j^{(2)} = \sum_{l=-N/2}^{N/2-1} \left[ \widehat{u}_l^{(1)} \exp(-i\tau k|\nu_l|^\alpha) \right] e^{i\nu_l(x_j-a)}, \quad 0 \leq j \leq N, \quad n \geq 0, \tag{8.8.22}$$

$$u_j^{(n+1)} = u_j^{(2)} \exp \left\{ -i\frac{k}{2} [\gamma(x_j) + \beta|u_j^{(2)}|^{2\delta}] \right\}, \tag{8.8.23}$$

where  $u_j^n$  represents the numerical approximation of  $u(x_j, t_n)$ . With  $n = 0$ , we get  $u_j^0 = u_0(x_j)$ ,  $0 \leq j \leq N$ . Readers are referred to [43, 74] for a more general discussion on the splitting method.

In the same fashion, the powers  $(-\Delta)^{\alpha/2}$  of the operator  $(-\Delta)$ , in  $\Omega$  with zero Dirichlet or Neumann boundary data, are given via the spectral representation by adopting the powers of the eigenvalues of the major operator. Assuming  $(\varphi_j, \lambda_j)$  are the eigenfunctions and eigenvectors of  $(-\Delta)$  in  $\Omega$  with either zero Dirichlet or Neumann boundary conditions. In fact, we can define the fractional Laplacian  $(-\Delta)^{\alpha/2}$  in the space of functions

$$S_0^{\alpha/2}(\Omega) = \left\{ u = \sum_{j=0}^{\infty} a_j \lambda_j^{\alpha/2} \in L^2(\Omega) : \|u\|_{S_0^{\alpha/2}(\Omega)} = \left( \sum_{j=0}^{\infty} a_j^2 \lambda_j^{\alpha/2} \right)^{1/2} < \infty \right\}, \tag{8.8.24}$$

where

$$\|u\|_{S_0^{\alpha/2}(\Omega)} = \|(-\Delta)^{\alpha/4} u\|_{L^2(\Omega)}. \tag{8.8.25}$$

Therefore, for any  $u \in S_0^{\alpha/2}$ , the Laplacian  $(-\Delta)^{\alpha/2}$  is defined by

$$(-\Delta)^{\alpha/2} u = \sum_{i=0}^{\infty} a_i \lambda_i^{\alpha/2} \varphi_i, \tag{8.8.26}$$

where  $\varphi_j$  and  $\lambda_j$  will depend on the specified boundary conditions. For the homogeneous Neumann boundary condition, we have

$$(\varphi_j, \lambda_j) = \left( \left[ \frac{\pi j}{b-a} \right]^2, \sqrt{\frac{2}{b-a}} \sin \left[ \frac{(x-a)\pi j}{b-a} \right] \right), \tag{8.8.27}$$

and for the homogeneous Dirichlet boundary condition, we get

$$(\varphi_j, \lambda_j) = \left( \left[ \frac{(j+1)\pi}{b-a} \right]^2, \sqrt{\frac{2}{b-a}} \sin \left[ \frac{(x-a)\pi(j+1)}{b-a} \right] \right). \quad (8.8.28)$$

This technique results in a full diagonal representation of the fractional operator with orders  $0 < \alpha \leq 1$  or  $1 < \alpha \leq 2$ , and achieves spectral accuracy regardless of the chosen value of  $\alpha$ . This method can be extended to high spatial dimensions. To present this method, we use the fast Fourier transform (FFT) to (8.8.15), so that

$$i u_t = \tau (\Delta^{\alpha/2}) u + f(u), \quad (8.8.29)$$

where  $f(u) = \gamma(x)u + \beta|u|^{2\delta}$ . To give 2D representation of (8.8.29) in Fourier space, we have

$$U_t(\chi_x, \chi_y, t) = -\tau (\chi_x^{\alpha/2} + \chi_y^{\alpha/2}) U(\chi_x, \chi_y, t) + \mathcal{F}[f(u(x, y, t))], \quad (8.8.30)$$

where  $U$  is the double Fourier transforms of function  $u(x, y, t)$ . In other words,

$$\mathcal{F}[u(x, y, t)] = U(\chi_x, \chi_y, t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} u(x, y, t) e^{-i(\chi_x x + \chi_y y)} dx dy. \quad (8.8.31)$$

To completely remove the issue of stiffness in the fractional Laplacian operator using integrating factors, we let  $\Omega^{\alpha/2} = (\chi_x^{\alpha/2} + \chi_y^{\alpha/2})$ , and set

$$U = e^{-\tau \Omega^{\alpha/2} t} \bar{U},$$

so that we now left with

$$\partial_t \bar{U} = e^{-\tau \Omega^{\alpha/2} t} \mathcal{F}[f(u)]. \quad (8.8.32)$$

Next, we discretize the square domain  $N_x$  and  $N_y$  in the spatial directions of  $x$  and  $y$ . We utilize the discrete fast Fourier transform (DFFT) [63] to transform (8.8.32) to an ODE in the form

$$\partial_t \bar{U}_{i,j} = e^{-\tau \Omega_{i,j}^{\alpha/2} t} \mathcal{F}[f(u_{i,j})], \quad (8.8.33)$$

where  $u_{i,j} = u(x_i, y_j)$  and  $\Omega_{i,j}^{\alpha/2} = (\chi_x^{\alpha/2}(i) + \chi_y^{\alpha/2}(j))$ . Boundary conditions are now fixed at extreme ends of the computational domain. Any explicit time-solver can be applied to advance in time. Here, we apply the improved version of Cox–Matthews [15, 27, 65] exponential time-differencing Runge–Kutta method.

$$\begin{aligned}
\mathcal{U}_{n+1} = & e^{\mathbf{L}h}\mathcal{U}_n + h[4\varphi_3(\mathbf{L}h) - 3\varphi_2(\mathbf{L}h) + \varphi_1(\mathbf{L}h)]\mathbf{F}(u_n, v_n, t_n) \\
& + 2h[\varphi_2(\mathbf{L}h) - 2\varphi_3(\mathbf{L}h)]\mathbf{F}(\mu_2, t_n + h/2) \\
& + 2h[\varphi_2(\mathbf{L}h) - 2\varphi_3(\mathbf{L}h)]\mathbf{F}(\mu_3, t_n + h/2) \\
& + h[\varphi_3(\mathbf{L}h) - 2\varphi_2(\mathbf{L}h)]\mathbf{F}(\mu_4, t_n + h),
\end{aligned} \tag{8.8.34}$$

with the stages  $\mu_i$  given as

$$\begin{aligned}
\mu_2 &= e^{\mathbf{L}h/2}\mathcal{U}_n + (\mathbf{L}h/2)\varphi_1(\mathbf{L}h/2)\mathbf{F}(u_n, v_n, t_n) \\
\mu_3 &= e^{\mathbf{L}h/2}\mathcal{U}_n + (\mathbf{L}h/2)[\varphi_1(\mathbf{L}h/2) - 2\varphi_2(\mathbf{L}h/2)]\mathbf{F}(u_n, v_n, t_n) + h\varphi_2(\mathbf{L}h/2)\mathbf{F}(\mu_2, t_n + h/2) \\
\mu_4 &= e^{\mathbf{L}h}\mathcal{U}_n + h[(\varphi_1(\mathbf{L}h) - 2\varphi_2(\mathbf{L}h))\mathbf{F}(u_n, v_n, t_n) + 2h\varphi_2(\mathbf{L}h)\mathbf{F}(\mu_3, t_n + h)],
\end{aligned}$$

with functions  $\varphi_{1,2,3}$  defined as

$$\varphi_1(z) = \frac{e^z - 1}{z}, \quad \varphi_2 = \frac{e^z - 1 - z}{z^2}, \quad \varphi_3 = \frac{e^z - 1 - z - z^2/2}{z^3}.$$

Readers are referred to [15, 27, 58, 61, 62, 64] for detailed derivation and stability of the ETD4RK method.

## 8.9 Numerical Experiments

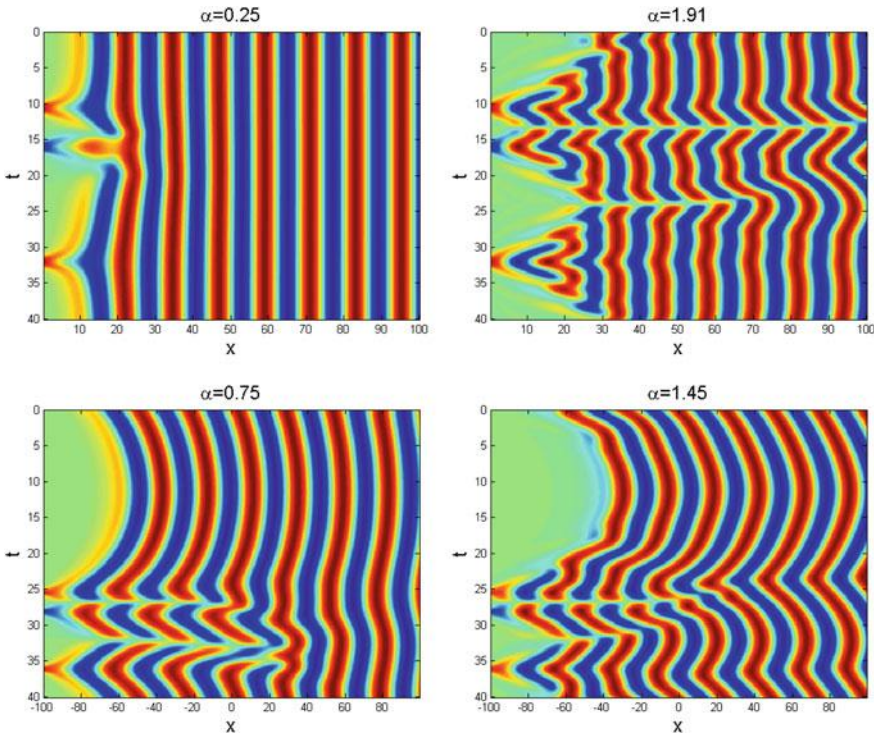
In this section, we experiment the dynamics of the fractional-in-space nonlinear Schrödinger equation (8.8.1) with harmonic potential in (8.8.2) in one, two and three dimensions as follows.

### 8.9.1 One-Dimensional Results for Fractional Schrödinger Equation

We examine the dynamics of fractional Schrödinger equation (8.8.1) with harmonic potential  $P(x) = 0.5(x^2)$  subject to initial condition

$$u(x, 0) = \exp[-20(x - \epsilon/3)^2/\epsilon] - \exp[-20(x - \epsilon/2)^2/\epsilon] + \exp[-20(x - \epsilon)^2/\epsilon] \tag{8.9.1}$$

on two different domains  $\Omega = [0, L]$  and  $\Omega = [-L, L]$ .

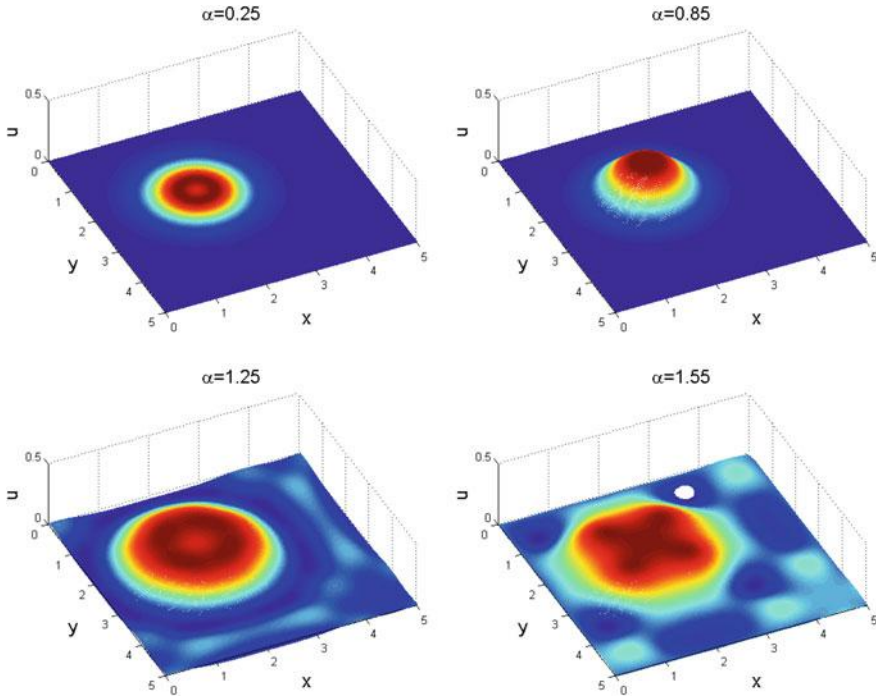


**Fig. 8.65** 1D evolution of the wave function  $|u(x, t)|$  of the fractional Schrödinger equation (8.8.1) for  $\beta = -1.3$  with a harmonic potential  $P(x) = 0.5x^2$ , for different instances of  $\alpha$  and  $\epsilon = 100$  with final time  $t = 40$ . The computational domains are  $x \in [0, L]$  and  $x \in [-L, L]$ ,  $L = 100$  for upper and lower rows, respectively

In Fig. 8.65, we observed different evolutions of the wave function  $|u(x, t)|$  for different values of  $\alpha$  and harmonic potential  $P(x) = 0.5x^2$ . The upper and lower plots correspond to the computational domain  $x \in [0, L]$  and  $x \in [-L, L]$ , respectively. The contour results are clear evidence that the wave function oscillates in both domains. Columns 1 and 2 correspond to sub-diffusive and superdiffusive results.

### 8.9.2 Two-Dimensional Results for Fractional Schrödinger Equation

We now extend to 2D dynamics of the fractional Schrödinger equation (8.8.1) with the harmonic potential given as  $P(x, y) = 0.5(x^2 + y^2)$ . We experiment with the



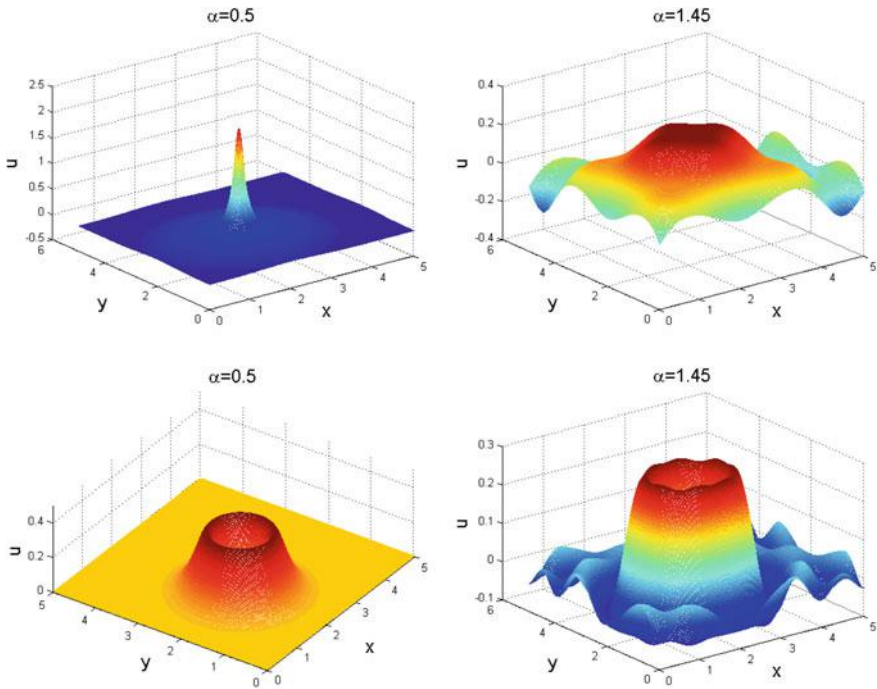
**Fig. 8.66** 2D Distribution of the wave function  $|u(x, y, t)|$  in the fractional Schrödinger equation (8.8.1) for  $\beta = 0$  with a harmonic potential  $V(x, y) = 0.5(x^2 + y^2)$ , at some instances of fractional power  $\alpha = 0.25, 0.75, 1.25, 1.55, \mu = 2$ . Simulation runs for  $N = 200$  and final time  $t = 2$

domain  $\Omega = [0, L] \times [0, L]$ ,  $L = 5$  with mesh size  $h_x = h_y = 0.05$  and time step  $k = 0.5$ . We simulate the 2D dynamics in Fig. 8.66 with the initial condition

$$u(x, y, 0) = \exp(-2(x - \mu)^2 + (y - \mu)^2). \tag{8.9.2}$$

We observed in Fig. 8.66 that the evolution of the wave function also oscillates in a cyclic manner and grows in the computational domain with increasing value of fractional order  $\alpha$ . As  $\alpha \rightarrow 2$ , the stable stationary solutions in Fig. 8.66 are fast becoming unstable spatiotemporal dynamic. The maximum computer time for these experiments is between 5 and 10 s.

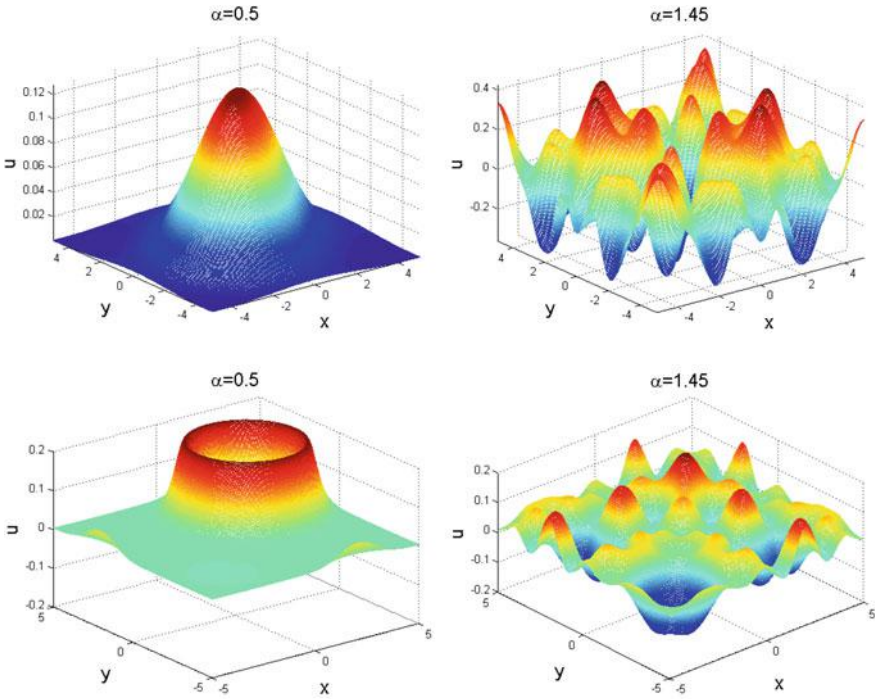
We present the 2D dynamics to (8.8.1) in the presence of the local interactions when  $\beta \neq 0$  as displayed in Figs. 8.67 and 8.68 for different boundary conditions. We experiment results in Fig. 8.67 with the same computational domain as in Fig. 8.66 different values of  $\alpha$ . The upper row corresponds to the focusing case if  $\beta > 0$  and



**Fig. 8.67** The 2D results for Eq. (8.8.1), showing the dynamic evolution for focusing (upper) and defocussing (lower) cases with  $\mu = 2$  and  $\beta = \pm 1.25$  on domain size  $(x, y) \in [0, 5] \times [0, 5]$  and final time  $t = 2$

lower row represents the defocussing type if  $\beta < 0$ . A chaotic pattern emerged when  $\alpha = 1.45$ , the dissipative structures here are similar to the ones obtained for the classical case, see [63].

In Fig. 8.68, we simulate with boundary domain size  $(x, y) \in [-5, 5] \times [-5, 5]$  and initial function (8.9.2) for some  $\alpha$  with  $\beta = \pm 1.25$  and a 2D harmonic potential  $P(x, y) = 0.5(x^2 + y^2)$ . Columns 1–2 correspond to  $\alpha = 0.5$  and  $\alpha = 1.45$ . The steady dissipative structures are obtained for both focusing and defocussing cases of subdiffusion model at  $\alpha = 0.5$ , but as for the superdiffusive scenario, when  $1 < \alpha \leq 2$  we observed spurious chaotic and non-stationary structures for both focusing and defocussing cases, as evident in column 2 of Fig. 8.68.



**Fig. 8.68** 2D evolution  $|u(x, y, t)|$  for Eq.(8.8.1) with domain size  $(x, y) \in [-5, 5] \times [-5, 5]$ ,  $\mu = 2$  and initial condition (8.9.2). The upper and lower surface plots are obtained for focusing ( $\beta = 1.25$ ) and defocussing ( $\beta = -1.25$ ) for different values of  $\alpha$

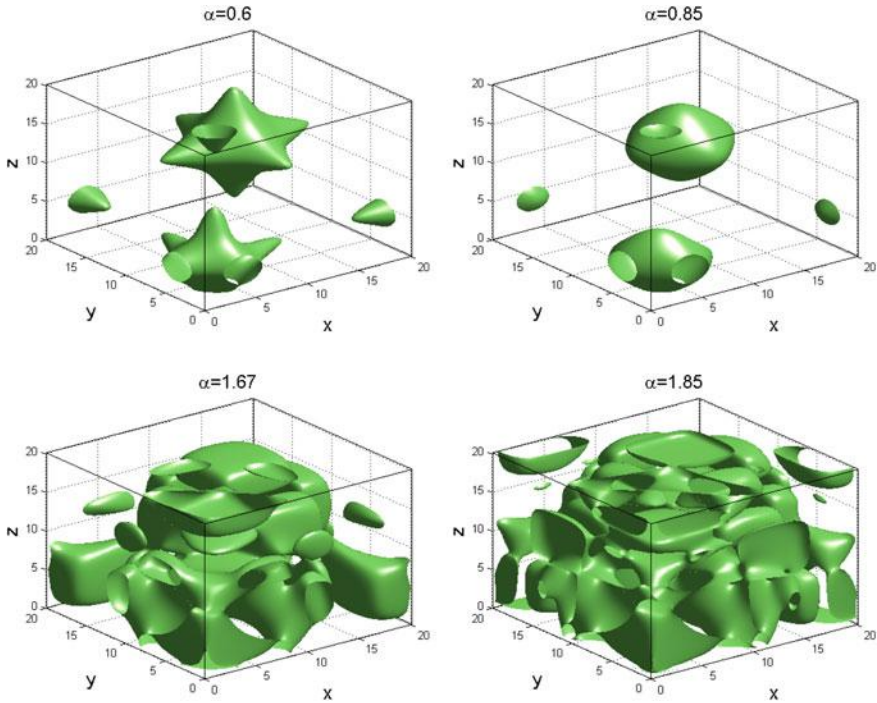
### 8.9.3 Three-Dimensional Results for Fractional Schrödinger Equation

With some modifications to the 2D program, we experiment the 3D dynamics of fractional Schrödinger equation (8.8.1). For this experiment, we utilize the initial condition

$$u(x, y, z, 0) = \exp(-20((x - \hbar)^2 + (y - \hbar)^2 + (z - \hbar)^2)), \tag{8.9.3}$$

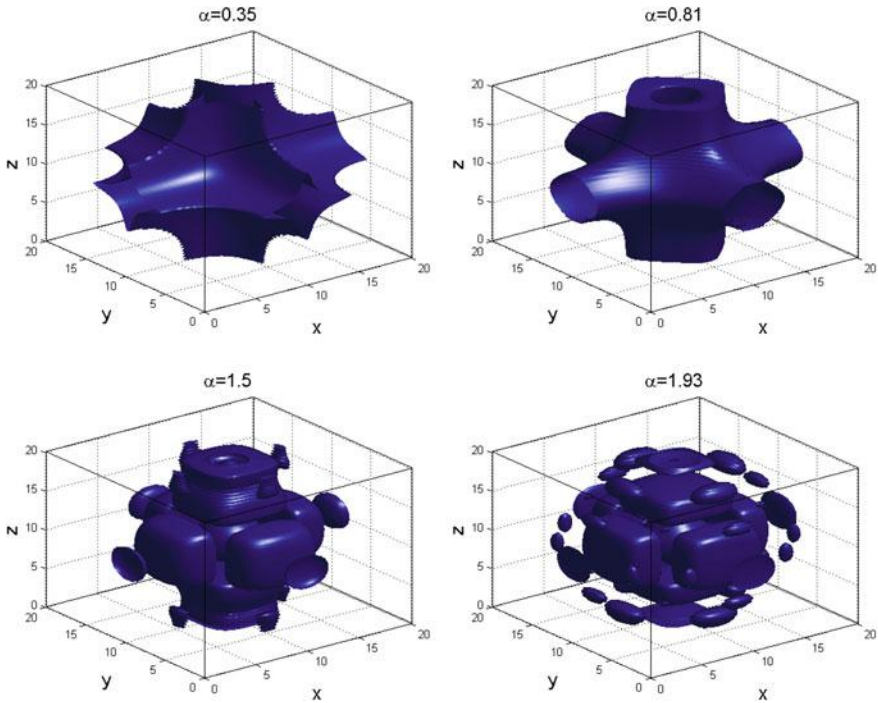
subject to the boundary conditions set at the extremes of computational domain  $(x, y, z) \in [0, L]^3$ .

In Figs.8.69 and 8.70, we observed different dynamics for the focusing and defocussing cases. We perform series of numerical simulations of the fractional Schrödinger equation (8.8.1) in 3D with a time step size of  $k = 0.05$  and space step



**Fig. 8.69** Focussing case: Showing the 3D distribution of function  $|u(x, y, z, t)|$  for Schrödinger Eq. (8.8.1) at  $\beta = 1.3, \hbar = 2$  with harmonic potential  $P(x, y, z) = 0.5(x^2 + y^2 + z^2)$ , for various  $\alpha$  in the interval  $0 < \alpha < 2$  and final time  $t = 10$

size  $h_x = h_y = h_z = 1.25$  and harmonic potential  $V(x, y, z) = 0.5(x^2 + y^2 + z^2)$ . We keep  $\hbar = 2, L = 20, \beta = \pm 1.3, t = 10$  and vary  $\alpha$  in the interval  $0 < \alpha \leq 2$ . In the focussing case (Fig. 8.69) in the subinterval  $0 < \alpha \leq 0.5$ , we observed that the wave function  $|u(x, y, z, t)|$  gives rise to chaotic patterns, and spreads from the origin along the axes  $(x, y, z) \in [0, L]^3$ . But as  $\alpha$  is increasing say from 0.5 to 1.55 in the interval  $0.5 < \alpha \leq 1.55$ , the waves evolve to form some familiar patterns such as star-like, dice-like or diamond shape. At  $1.55 < \alpha \leq 2$ , the wave function oscillates into a more chaotic structure. The structure formed for the defocussing case in Fig. 8.70 is assumed to have more interpretations and usage in physics and engineering, more complex (connector-like) structures emerge as the value of  $\alpha$  is increasing.



**Fig. 8.70** Defocussing 3D scenario for  $\beta = -1.3$ ,  $\hbar = 2$  showing spatiotemporal and chaotic evolutions of (8.8.1) with harmonic potential  $P(x, y, z) = 0.5(x^2 + y^2 + z^2)$ , for different  $\alpha$  in the interval  $0 < \alpha \leq 2$

## References

1. J. Al-Omari, S.A. Gourley, Monotone travelling fronts in an age-structured reaction-diffusion model of a single species. *J. Math. Biol.* **45**, 294–312 (2002)
2. B. Al-Saqabi, L. Boyadjiev, Y. Luchko, Comments on employing the Riesz-Feller derivative in the Schrödinger equation. *Eur. Phys. J. Spec. Topics* **222**, 1779–1794 (2013)
3. P. Amore, F.M. Fernández, C.P. Hofmann, R.A. Sáenz, Collocation method for fractional quantum mechanics. *J. Math. Phys.* **51**, 122101 (2010)
4. A. Atangana, On the new fractional derivative and application to nonlinear Fisher's reaction-diffusion equation. *Appl. Math. Comput.* **273**, 948–956 (2016)
5. A. Atangana, *Derivative with a New Parameter: Theory, Methods and Applications* (Academic Press, New York, 2016)
6. A. Atangana, *Fractional Operators with Constant and Variable Order with Application to Geo-Hydrology* (Academic Press, New York, 2017)
7. A. Atangana, R.T. Alqahtani, Numerical approximation of the space-time Caputo-Fabrizio fractional derivative and application to groundwater pollution equation. *Adv. Differ. Equ.* **2016**(1), 1–13 (2016)
8. A. Atangana, J.J. Nieto, Numerical solution for the model of RLC circuit via the fractional derivative without singular kernel. *Adv. Mech. Eng.* **7**, 1–6 (2015)
9. M.D. Bramson, Maximal displacement of branching brownian motion. *Commu. Pure Appl. Math.* **31**, 531–581 (1978)

10. P.K. Brazhnik, J.J. Tyson, On traveling wave solutions of Fisher's equation in two spatial dimensions. *SIAM J. Appl. Math.* **60**, 371–391 (2000)
11. N.F. Britton, *Reaction-Diffusion Equations and Their Applications to Biology* (Academic Press, London, 1986)
12. A. Bueno-Orovio, D. Kay, K. Burrage, Fourier spectral methods for fractional-in-space reaction-diffusion equations. *BIT Numer. Math.* **54**, 937–954 (2014)
13. M. Caputo, M. Fabrizio, A new definition of fractional derivative without singular kernel. *Prog. Fract. Differ. Appl.* **1**, 73–85 (2015)
14. C. Celik, M. Duman, Crank-Nicolson method for the fractional diffusion equation with the Riesz fractional derivative. *J. Comput. Phys.* **231**, 1743–1750 (2012)
15. S.M. Cox, P.C. Matthews, Exponential time differencing for stiff systems. *J. Comput. Phys.* **176**, 430–455 (2002)
16. A. Doelman, T.J. Kaper, P.A. Zegeling, Pattern formation in the one-dimensional Gray-Scott model. *J. Nonlinear Sci.* **10**, 523–563 (1997)
17. Z. Feng, Traveling wave behavior for a generalized fisher equation. *Chaos Solitons Fract.* **38**, 481–488 (2008)
18. P.C. Fife, *Mathematical Aspects of Reacting and Diffusing systems*, vol. 28 (Lecture Notes in Biomathematics (Springer, New York, 1979))
19. R.A. Fisher, The wave of advance of advantageous genes. *Ann. Eugen.* **7**, 353–369 (1937)
20. S.A. Gourley, Travelling front solutions of a nonlocal Fisher equation. *J. Math. Biol.* **41**, 272–284 (2000)
21. P. Gray, S.K. Scott, Autocatalytic reactions in the isothermal, continuous stirred tank reactor: Isolates and other forms of multistability. *Chem. Eng. Sci.* **38**, 29–43 (1983)
22. P. Gray, S.K. Scott, Autocatalytic reactions in the isothermal, continuous stirred tank reactor: oscillations and instabilities in the system  $A + 2B \rightarrow 3B; B \rightarrow C$ . *Chem. Eng. Sci.* **39**, 1087–1097 (1984)
23. S. Hamdi, W.E. Schiesser, G.W. Griffiths, Method of lines. *Scholarpedia* **2**(7), 2859 (2010)
24. E. Hanert, A comparison of three Eulerian numerical methods for fractional-order transport models. *Environ. Fluid Mech.* **10**, 7–20 (2010). <https://doi.org/10.1007/s10652-009-9145-4>
25. E. Hanert, On the numerical solution of space-time fractional diffusion models. *Comput. Fluids* **46**, 33–39 (2011)
26. D.A.F. Kamenetskii, *Diffusion and Heat Exchange in Chemical Kinetics* (Princeton University Press, Princeton, NJ, 1955)
27. A.K. Kassam, L.N. Trefethen, Fourth-order time-stepping for stiff PDEs. *SIAM J. Sci. Comput.* **26**, 1214–1233 (2005)
28. M.M. Khader, On the numerical solutions for the fractional diffusion equation. *Commun. Nonlinear Sci. Numer. Simul.* **16**, 2535–2542 (2010)
29. A.A. Kilbas, H. YuF Luchko, J.J. Trujillo, Martínez, Fractional Fourier transform in the framework of fractional calculus operators. *Integral Transforms Spec. Funct.* **21**, 779–795 (2010)
30. A.A. Kilbas, H.M. Srivastava, J.J. Trujillo, *Theory and Applications of Fractional Differential Equations* (Elsevier, Amsterdam, 2006)
31. A.N. Kolmogorov, I.G. Petrovskii, N.S. Piskunov, A study of diffusion equation with increase in the quantity of matter and its application to a biological problem. *Mosc. Univ. Bull. Math.* **1**, 1–25 (1937)
32. M. Kot, Discrete-time travelling waves: ecological examples. *J. Math. Biol.* **30**, 413–436 (1992)
33. M. Kot, *Elements of Mathematical Ecology* (Cambridge University Press, Cambridge, 2001)
34. M. Kot, W.M. Schaffer, Discrete-time growth-dispersal models. *Math. Biosci.* **80**, 109–136 (1986)
35. S. Krogstad, Generalized integrating factor methods for stiff PDEs. *J. Comput. Phys.* **203**, 72–88 (2005)
36. Y.N. Kyrchko, K.B. Blyuss, Persistence of travelling waves in a generalized Fisher equation. *Phys. Lett. A* **373**, 668–674 (2009)

37. N. Laskin, Fractional Schrödinger equations. *Phys. Rev. E* **66**, 056108 (2002)
38. X. Li, C. Xu, Existence and uniqueness of the weak solution of the space-time fractional diffusion equation and a spectral method approximation. *Commun. Comput. Phys.* **8**, 1016–1051 (2010)
39. A. Liemert, A. Kienle, Fractional Schrödinger equation in the presence of the linear potential. *Mathematics* **4**(31) (2016). <https://doi.org/10.3390/math4020031>
40. Y. Luchko, Fractional Schrödinger equation for a particle moving in a potential well. *J. Math. Phys.* **54**, 012111 (2013)
41. Y. Luchko, Fractional wave equation and damped waves. *J. Math. Phys.* **54**, 031505 (2013)
42. Y. Luchko, Wave-diffusion dualism of the neutral-fractional processes. *J. Comput. Phys.* **293**, 40–52 (2015)
43. G. Marchuk, *Splitting and Alternating Direction Methods, in Handbook of Numerical Analysis* (North Holland, Amsterdam, 1990)
44. M.M. Meerschaert, C. Tadjeran, Finite difference approximations for fractional advection-dispersion ow equations. *J. Comput. Appl. Math.* **172**, 65–77 (2004)
45. M.M. Meerschaert, C. Tadjeran, Finite difference approximations for two-sided space-fractional partial differential equations. *Appl. Numer. Math.* **56**, 80–90 (2006)
46. M.M. Meerschaert, H.P. Scheffler, C. Tadjeran, Finite difference methods for two-dimensional fractional dispersion equation. *J. Comput. Phys.* **211**, 249–261 (2006)
47. J.D. Murray, *Lectures on Non-linear Differential Equations Models in Biology* (Oxford University Press, London, 1977)
48. J.D. Murray, *Mathematical Biology* (Springer, Berlin, 1989)
49. J.D. Murray, *Mathematical Biology, 19: Biomathematics Texts* (Springer, Berlin, 1993)
50. J.D. Murray, *Mathematical Biology II: Spatial Models and Biomedical Applications* (Springer-Verlag, Berlin, 2003)
51. J.D. Murray, *Mathematical Biology I: An Introduction* (Springer, New York, 2003)
52. Z.M. Odibat, S. Momani, Application of variational iteration method to nonlinear differential equation of fractional order. *Int. J. Nonlinear Sci. Numer. Simul.* **7**, 27–34 (2006)
53. K.B. Oldham, J. Spanier, *The Fractional Calculus: Theory and Applications of Differentiation and Integration to Arbitrary Order* (Dover Publication, New York, 2006)
54. M.D. Ortigueira, *Fractional Calculus for Scientists and Engineers* (Springer, New York, 2011)
55. K.M. Owolabi, Efficient numerical simulation of non-integer-order space-fractional reaction-diffusion equation via the Riemann-Liouville operator. *Eur. Phys. J. Plus* **133**, 98 (2018). (16 pages). <https://doi.org/10.1140/epjp/i2018-11951-x>
56. K.M. Owolabi, Robust IMEX schemes for solving two-dimensional reaction-diffusion models. *Int. J. Nonlinear Sci. Numer. Simul.* **16**, 271–284 (2015). <https://doi.org/10.1515/ijnsns-2015-0004>
57. K.M. Owolabi, Mathematical analysis and numerical simulation of patterns in fractional and classical reaction-diffusion systems. *Chaos Solitons Fractals* **93**, 89–98 (2016)
58. K.M. Owolabi, *Efficient Numerical Methods for Reaction-Diffusion Problems* (Saarbrücken, Deutschland/Germany, 2016)
59. K.M. Owolabi, Robust and adaptive techniques for numerical simulation of nonlinear partial differential equations of fractional order. *Commun. Nonlinear Sci. Numer. Simul.* **44**, 304–317 (2017)
60. K.M. Owolabi, A. Atangana, Numerical solution of fractional-in-space nonlinear Schrödinger equation with the Riesz fractional derivative. *Eur. Phys. J. Plus* **131**, 335 (2016). <https://doi.org/10.1140/epjp/i2016-16335-8>
61. K.M. Owolabi, K.C. Patidar, Higher-order time-stepping methods for time-dependent reaction-diffusion equations arising in biology. *Appl. Math. Comput.* **240**, 30–50 (2014)
62. K.M. Owolabi, K.C. Patidar, Numerical solution of singular patterns in one-dimensional Gray-Scott-like models. *Int. J. Nonlinear Sci. Numer. Simul.* **15**, 437–462 (2014). <https://doi.org/10.1515/ijnsns-2013-0124>
63. K.M. Owolabi, K.C. Patidar, Existence and permanence in a diffusive KiSS model with robust numerical simulations. *Int. J. Differ. Equ.* **2015**(485860), 8 (2015). <https://doi.org/10.1155/2015/485860>

64. K.M. Owolabi, K.C. Patidar, Numerical simulations of multicomponent ecological models with adaptive methods. *Theor. Biol. Med. Model.* **13**, 1 (2016). <https://doi.org/10.1186/s12976-016-0027-4>
65. K.M. Owolabi, K.C. Patidar, Effect of spatial configuration of an extended nonlinear Kierstead-Slobodkin reaction-transport model with adaptive numerical scheme. *Springer Plus* **5**, 303 (2016). <https://doi.org/10.1186/s40064-016-1941-y>
66. J.E. Pearson, Complex patterns in a simple system. *Science* **261**(1993), 189–192 (1993)
67. E. Pindza, K.M. Owolabi, Fourier spectral method for higher order space fractional reaction-diffusion equations. *Commun. Nonlinear Sci. Numer. Simul.* **40**, 112–128 (2016)
68. A.R. Plastino, C. Tsallis, Nonlinear Schrödinger equation in the presence of uniform acceleration. *J. Math. Phys.* **54**, 041505 (2013)
69. I. Podlubny, *Fractional Differential Equations* (Academic Press, San Diego, 1999)
70. W.N. Reynolds, J.E. Pearson, S. Ponce-Dawson, Dynamics of self-replicating patterns in reaction diffusion systems. *Phys. Rev. Lett.* **72**, 1120–1123 (1994)
71. R. Riaza, Time-domain properties of reactive dual circuits. *Int. J. Circ. Theory Appl.* **34**, 317–340 (2006)
72. S.G. Samko, B. Ross, Integration and differentiation to a variable fractional order. *Integral Transforms Spec. Funct.* **1**, 277–300 (1993)
73. S. Samko, A. Kilbas, O. Marichev, *Fractional Integrals and Derivatives: Theory and Applications* (Gordon and Breach, Amsterdam, 1993)
74. G. Strang, On the construction and comparison of difference schemes. *SIAM J. Numer. Anal.* **5**, 506–517 (1968)
75. L.N. Trefethen, *Spectral Methods in MATLAB* (SIAM, Philadelphia, 2000)
76. J.A.C. Weideman, S.C. Reddy, A MATLAB differentiation suite. *Trans. Math. Softw.* **26**, 465–519 (2001)
77. F.A. Williams, *Combustion Theory* (Addison-Wesley, Reading, MA, 1965)
78. F. Zeng, F. Liu, C. Li, K. Burrage, I. Turner, V. Anh, A Crank-Nicolson ADI spectral method for a two-dimensional Riesz space fractional nonlinear reaction-diffusion equation. *SIAM J. Numer. Anal.* **52**, 2599–2622 (2014)
79. F. Zeng, C. Li, F. Liu, I. Turner, Numerical algorithms for time-fractional subdiffusion equation with second-order accuracy. *SIAM J. Sci. Comput.* **37**, A55–A78 (2015)
80. Y. Zhang, X. Liu, M.R. Belić, W. Zhong, Y. Zhang, M. Xiao, Propagation dynamics of a light beam in a fractional Schrödinger equation. *Phys. Rev. Lett.* **115**, 180403 (2015)
81. M. Zheng, F. Liu, I. Turner, V. Anh, A novel high order space-time spectral method for the time fractional Fokker-Planck equation. *SIAM J. Sci. Comput.* **37**, A701–A724 (2015)

## Bibliography

82. B.S.T. Alkahtani, A. Atangana, Chaos on the Vallis model for El Niño with fractional operators. *Entropy* **18**(4) (2016) 17 pages. <https://doi.org/10.3390/e18040100>
83. H. Bahouri, J.Y. Chemin, R. Danchin, *Fourier Analysis and Nonlinear Partial Differential Equations* (Springer, Berlin, 2011)
84. A. Clout, J.F. Botha, A generalised groundwater flow equation using the concept of non-integer order derivatives. *Water SA* **32**, 1–7 (2006)
85. J.G. Charney, R. Fjörtoft, J. Von Neumann, Numerical integration of the barotropic vorticity equation. *Sven. Geofys. Fören.* **2**, 237–254 (1950)
86. R. Courant, K. Friedrichs, H. Lewy, On partial difference equations of mathematical physics. *IBM J. Res. Dev.* **11**, 215–234 (1967)
87. J. Crank, E. Nicolson, A practical method for numerical integration of solutions of partial differential equations of heat-conduction type. *Proc. Camb. Philos. Soc.* **43**, 50–67 (1963)

88. D.R. Durran, *Numerical Methods for Fluids Dynamics with Applications to Geophysics* (Springer Science+Business Media, New York, 2010)
89. E.F. Doungmo Goufo, Application of the Caputo-Fabrizio fractional derivative without singular kernel to Korteweg-de Vries-Burgers equation. *Math. Model. Anal.* **21**, 188–198 (2016)
90. B. Fornberg, Calculation of weights in finite difference formulas. *SIAM Rev.* **40**, 685–691 (1998)
91. S.D. Gedney, *Introduction to the Finite-Difference Time-Domain (FDTD)-Method for Electromagnetics* (Morgan and Claypool Publishers, Arizona, 2011)
92. J.D. Hoffman, *Numerical Methods for Engineers and Scientists* (Marcel Dekker Inc., New York, 2001)
93. H. Holden, K.H. Karlsen, *Nonlinear Partial Differential Equations* (Springer, Berlin, 2012). The Abel symposium
94. R.K. Jain, *Numerical Solution of Differential Equations*, 2nd edn. (Wiley Eastern Limited, New Delhi, 1984)
95. R.J. Leveque, *Finite Difference Methods for Ordinary and Partial Differential Equations* (SIAM, Philadelphia, 2007)
96. J. Liouville, Mémoire sur l'intégration de l'équation:  $(mx^2 + nx + p)d^2x/dx^2 + (qx + pr)dy/dx + sy = 0$  à l'aide des différentielles indices quelconques. *J. l'Ecole Roy. Polytechn.* **13**, 163–186 (1832)
97. J. Liouville, Mémoire sur le théorème des fonctions complémentaires. *J. Reine Angew. Math.* **11**, 119 (1934)
98. J. Liouville, Mémoire sur une formule d'analyse. *J. Reine Angew. Math.* **12**, 273–287 (1834)
99. J. Liouville, Mémoire sur le changement de la variable indépendante dans le calcul des différentielles indices quelconques. *J. l'Ecole Roy. Polytechn.* **15**, 1754 (1835)
100. J. Liouville, Mémoire sur l'usage que l'on peut faire de la formule de fourier, dan le calcul des différentielles à indices quelconques. *J. Reine Angew. Math.* **13**, 219–232 (1835)
101. J.H. Mathews, K.D. Fink, *Numerical Methods Using MATLAB* (Prentice Hall, New Jersey, 1999)
102. M. Riesz, Potentiels de divers ordres et leurs fonctions de Green. *C. R. Congrès Intern. Math.* **2**, 62–63 (1936)
103. M. Riesz, L'intégrales de Riemann-Liouville et potentiels. *Acta Litt. Acad. Sci. Szeged* **9**, 1–42 (1938)
104. G. Sewell, *The Numerical Solution of Ordinary and Partial Differential Equations* (Wiley, Hoboken, New Jersey, 2005)
105. J.W. Thomas, *Numerical Partial Differential Equations-Finite Difference Methods* (Springer, New York, 1995)
106. J.W. Thomas, *Numerical Partial Differential Equations: Conservation Laws and Elliptic Equations* (Springer, New York, 1999)
107. L.N. Trefethen, M. Embere, *Spectra and Pseudospectra: the Behavior of Nonnormal Matrices and Operators* (Princeton University Press, New Jersey, 2005)
108. G.K. Vallis, El Niño: a chaotic dynamical system? *Science* **232**, 243–255 (1986)