HIGH-ORDER DISCRETIZATION METHODS FOR FRACTIONAL DIFFUSION MODELS

The thesis submitted in partial fulfilment

for the Award of Degree

DOCTOR OF PHILOSOPHY

by

Deeksha Singh

DEPARTMENT OF MATHEMATICAL SCIENCES

INDIAN INSTITUTE OF TECHNOLOGY

(BANARAS HINDU UNIVERSITY)

VARANASI -221005

Roll No: 18121516 **October 2023**

CERTIFICATE

It is certified that the work contained in this thesis titled "***High-order discretization methods for fractional diffusion models***" by ***Deeksha Singh*** has been carried out under my supervision and that this work has not been submitted elsewhere for a degree.

It is further certified that the student has fulfilled all the requirements of Comprehensive Examination, Candidacy and SOTA for the award of Ph.D. degree.

30/10/2023

Dr. Rajesh Kumar Pandey
(Supervisor)
Associate Professor
Department of Mathematical Sciences
Indian Institute of Technology
(Banaras Hindu University)
Varanasi-221005

पर्यवेक्षक/Supervisor
गणितीय विज्ञान विभाग
Department of Mathematical Sciences
भारतीय प्रौद्योगिकी संस्थान
Indian Institute of Technology
(काशी हिन्दू विश्वविद्यालय)
(Banaras Hindu University)
वाराणसी/Varanasi-221005

DECLARATION BY THE CANDIDATE

I, ***Deeksha Singh***. certify that the work embodied in this thesis is my own bonafide work and carried out by me under the supervision of ***Dr. Rajesh Kumar Pandey*** from ***January, 2019*** to ***October, 2023*** at the ***Department of Mathematical Sciences, Indian Institute of Technology (Banaras Hindu University), Varanasi***. The matter embodied in this thesis has not been submitted for the award of any other degree/diploma. I declare that I have faithfully acknowledged and given credits to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not willfully copied any other's work, paragraphs, text, data, results, *etc.*, reported in journals, books, magazines, reports dissertations, theses, *etc.*, or available at websites and have not included them in this thesis and have not cited as my own work.

Date: 30/10/2023

Place: Varanasi

Deeksha Singh
(Deeksha Singh)

CERTIFICATE BY THE SUPERVISOR

It is certified that the above statement made by the student is correct to the best of my/our knowledge.

30/10/2023

(Dr. Rajesh Kumar Pandey)
Associate Professor
Department of Mathematical Sciences
Indian Institute of Technology
(Banaras Hindu University)
Varanasi-221005

पर्यवेक्षक/Supervisor
गणितीय विज्ञान विभाग
Department of Mathematical Sciences
भारतीय प्रौद्योगिकी संस्थान
Indian Institute of Technology
(काशी हिन्दू विश्वविद्यालय)
(Banaras Hindu University)
वाराणसी/Varanasi-221005

30.10.2023

(Prof. S. K. Pandey)
Professor and Head
Department of Mathematical Sciences
Indian Institute of Technology
(Banaras Hindu University)
Varanasi-221005

विभागाध्यक्ष/HEAD
गणितीय विज्ञान विभाग
Department of Mathematical Sciences
भारतीय प्रौद्योगिकी संस्थान
Indian Institute of Technology
(काशी हिन्दू विश्वविद्यालय)
(Banaras Hindu University)
वाराणसी/Varanasi-221005

COPYRIGHT TRANSFER CERTIFICATE

Title of the Thesis: *High-order discretization methods for fractional diffusion models*

Name of the Student: *Deeksha Singh*

Copyright Transfer

The undersigned hereby assigns to the Indian Institute of Technology (Banaras Hindu University), Varanasi all rights under copyright that may exist in and for the above thesis submitted for the award of the Ph.D. degree.

Date: 30/10/2023

Place: Varanasi

Deeksha Singh

(Deeksha Singh)

Note: However, the author may reproduce or authorize others to reproduce material extracted verbatim from the thesis or derivative of the thesis for author's personal use provided that the source and the Institute copyright notice are indicated.

TO

The Loving Memory of My Grandparents

Late Mrs. Indiravati Singh

&

Late Mr. Radheyshyam Singh

ACKNOWLEDGEMENTS

It gives me immense pleasure that I have an opportunity to express my sincere gratitude to all the people whose motivational influences helped me throughout this journey in obtaining my doctoral degree. This journey would not have been possible without the support, encouragement, and assistance of many individuals, and it is a mere attempt to name a few.

Fore mostly, I am gratefully indebted to my supervisor, **Dr. Rajesh Kumar Pandey**, Associate Professor, Department of Mathematical Sciences, IIT(BHU), Varanasi. His resilience and unrelenting enthusiasm inspire me. It has been a great honor to have had the opportunity to work with him. Besides his mathematical intelligence and teaching excellence, he has taught me things that are beyond books. Without his dedicated support and guidance, this dissertation would not have been possible. Really, he has been a friend, mentor, and critic who always ensured to shell out the best of me.

I express my cordial thanks to **Prof. S. K. Pandey**, the Head of the Department, for his support throughout my research work. I am highly obliged to all the faculty members of the Department of Mathematical Sciences for their support and encouragement. I express my sincere thanks to my RPEC members **Dr. Rajeev** and **Dr. Amitesh Kumar**, Department of Mechanical Engineering, for their helpful questions, comments, and constant feedback during the progress of my research work. I express my gratitude to the Director, Registrars, Deans, Heads, and Student Alumni of the Indian Institute of Technology (BHU), Varanasi. This journey of five years will be an inseparable part of my life because I have been groomed here.

I would like to extend a special thanks to **Dr. Swati Yadav** and **Dr. Kamlesh Kumar** for their constant motivation and support throughout this journey. I am also thankful to my seniors **Dr. Prashant Kumar Pandey**, **Dr. Sandeep**, **Ms. Pratima** and other lab mates **Ms. Farheen Sultana**, **Ms. Sarita Kumari**, **Ms. Eti Goel**, **Mr. Divyansh**, **Mr. Varun Makkar**, **Ms. Arya Tiwari**, **Ms. Riya** and **Ms. Sandhya** for their cooperation. Further, I am grateful to my close friends

Ms. Anshima Singh, **Ms. Anshika Pandey** and **Ms. Shivani Singh** for their emotional and intellectual support and for providing a listening ear and a comforting presence during stressful times.

I am also grateful to my Institute, IIT(BHU), for providing the necessary resources throughout my research. Also, the versatile qualities I developed here are going to remain with me throughout my life. I express my thanks to all non-teaching staff members of the Department for their support. I gratefully acknowledge the University Grant Commission (UGC), India, for providing the fellowships in the form of Junior Research Fellowship and Senior Research fellowship.

My family has been my pillar of strength throughout this journey. I owe a debt of gratitude to my Parents **Mrs. Laxmi Singh** and **Mr. Arvind Kumar Singh** for their unwavering support, patience, and encouragement throughout this demanding endeavor. Their belief in me kept me motivated during challenging times. Words are insufficient to express my profound sense of gratitude to my siblings **Mr. Dhananjay Singh** and **Ms. Shraddha Singh**, who always stood by my decisions and provided all kinds of support and morals. I would like to take a moment to express my deep appreciation and gratitude to my extended family, my Aunts and Uncles, **Mrs. Shashi Singh**, **Mr. Arun Kumar Singh**, **Mrs. Neelam Singh**, **Mr. Akhilesh Singh**, my cousins, **Mr. Anand Kumar Singh**, **Ms. Arpita Singh**, **Mr. Aditya Singh**, and my sister-in-law **Mrs. Arpita Singh**. While you may not have been directly involved in this journey, your presence and support have been an integral part of my success.

I dedicate this thesis to the loving memory of my dear Grandparents, **Late Mr. Radheyshyam Singh** and **Late Mrs. Indiravati Singh**, whose unwavering love, wisdom, and encouragement have been a constant source of inspiration throughout my life. Their wisdom and guidance have shaped my character and fueled my passion for learning.

This acknowledgment would be incomplete if the name of great visionary **Pt. Madan Mohan Malaviya** is not mentioned who made this divine center of knowledge. Deepest regards to him.

In the completion of this thesis, I humbly acknowledge the presence and guidance of the Divine Creator, whose wisdom, grace, and providence have been a constant source of strength and inspiration throughout my academic journey.

Deeksha Singh

Symbols

u	solute concentration
V	average fluid velocity
K	diffusion coefficient
x	independent variable in x-direction
y	independent variable in y-direction
t	independent variable in time-direction
$\mathcal{O}$	big O
α	fractional order (non integer)
$E_{\alpha,\beta}$	two parameter Mittag-Leffler function
$E^{\gamma}_{\alpha,\beta}$	three parameter Mittag-Leffler function
h	spatial step-size
τ	temporal step-size
$M,\ N,\ M_1,\ M_2$	number of subintervals
F	source function or unknown function
f	reaction function
$I^{\alpha}_{a^+}$	Riemann-Liouville fractional integral of order α
${}^{RL}_{a}D^{\alpha}_{t}$	Riemann-Liouville fractional derivative of order α
${}^{C}_{a}D^{\alpha}_{t}$	Caputo fractional derivative of order α
$I^{\gamma}_{\rho,\alpha,\omega,a}$	Prabhakar integral of order α
${}^{\mathrm{RLP}}_{a}D^{\gamma}_{\rho,\alpha,\omega}$	Riemann-Liouville Prabhakar derivative of order α
${}^{\mathrm{CP}}_{a}D^{\gamma}_{\rho,\alpha,\omega}f(t)$	Caputo Prabhakar derivative of order α
MAE	maximum absolute error
MAE_2	error in L_2 norm
CO	convergence order

Contents

List of Figures

List of Tables