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Wavelet Solutions for Reaction–Diffusion Problems in Science and Engineering

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Dedicated
With Love and Regards to
My Parents and Wife

Preface

The primary intention of this book is to examine the efficiency of various wavelet methods when applied to multiple problems of nonlinear and fractional-order reaction–diffusion equations of substantial importance. Having an easy-to-fallow scientific insight and being sufficiently realistic for studying important design problems, reaction–diffusion models of enzyme kinetics play an important role in chemical kinetics theory. The characterizing equations of enzyme kinetics models are highly nonlinear reaction–diffusion equations which do not have analytical solutions. As existing methods can only handle a limited range of these equations, many computational methods have been developed in recent years, having either equal or better performance. In general, the qualitative behavior of the solutions may not always be fully exposed by semi-analytical method results. In order to achieve this goal, discrete wavelet transform is studied first, followed by their properties, convergence, and computational complexity for addressing a few issues of enzyme kinetics. Therefore, this book investigates theoretically a few steady- and unsteady- state reaction–diffusion problems arising in enzyme kinetics models.

Wavelet method is a recently developed tool in applied mathematics. Investigation of various wavelet methods for their capability of analyzing various dynamic phenomena has gained more attention in engineering research. Starting from offering good solutions for differential equations to capturing the nonlinearity in data distribution, wavelets are used as appropriate tools at various places to provide a decent mathematical model for scientific phenomena, usually modeled through linear or nonlinear differential equations. Review shows that the wavelet method is efficient and powerful in solving wide class of linear and nonlinear reaction–diffusion equations. This book also intends to provide great utility of wavelets to science and engineering problems which owe its origin to 1919.

Chapters maintain a balance between mathematical rigor and practical applications of wavelet theory, thereby, catering to students and researchers with particular needs, wanting to understand not only the reaction–diffusion problems but also wavelets theory in order to have a broader understanding. Operational matrices have been introduced to convert the given nonlinear and fractional differential equations into a system of nonlinear algebraic equations. Applications of Haar, Legendre, and Chebyshev wavelet methods and wavelet-based hybrid methods in the field of nonlinear and fractional-order reaction–diffusion equations are also included for the first time. This book also includes innovative techniques for finding the approximate solutions of highly nonlinear boundary value problems. Wavelet-based methods have been used to combine the strength of both analytical and numerical methods to produce efficient hybrid techniques.

When compared to other numerical methods of solutions, discrete wavelet transforms (Haar, Legendre and Chebyshev) have some preferences such as mathematical efficiency, simplicity, and possibility to implement standard algorithms and high accuracy for a small number of grid points. Solutions based on the wavelet methods are usually simpler and faster than in case of other methods. For these reasons, wavelets have obtained greater popularity and the number of papers about discrete wavelets is rapidly increasing. For a reader, it is difficult to find his way among a large number of publications.

Therefore, a book like this, explaining the applications of the discrete wavelet transform in calculus, is extremely necessary. As different variants of the wavelet methods exist, it is not reasonable to handle and analyze all of them in detail. Therefore, we have decided to choose a method of solution, which is sufficiently universal and is applicable to solve all the problems by a unit approach. Other treatments will be referred to and discussed in the section-related papers added to each chapter. To demonstrate the efficiency and accuracy of the proposed method, a number of examples are solved. Mostly test problems, for which the exact solution or solution obtained by other methods is known, are considered.

The book is meant for researchers, teachers, and students of applied mathematics, physics, engineering, and related disciplines. To make the book accessible for a wider circle of readers, some mathematical finesse is left out.

Thanjavur, Tamil Nadu, India Dr. G. Hariharan

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I have received considerable assistance from my colleagues in the Department of Mathematics, SASTRA University. Moreover, I am especially grateful to the team of Springer for cooperation in all aspects of the production of the book.

I thank my parents for their blessings. Last but not least, I thank my wife and my daughters for their patience and support.

I am looking forward to receiving comments and suggestions on this work from students, teachers, and researchers.

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About the Author

G. Hariharan has been Senior Assistant Professor at the Department of Mathematics, SASTRA University, Thanjavur, Tamil Nadu, India, since 2003. He previously served as a lecturer at Adhiparasakthi Engineering College, Melmaruvathur, Tamil Nadu. Dr. Hariharan received his MSc and PhD degrees in Mathematics from Bharathidasan University, Trichy, and SASTRA University, in 1999 and 2010, respectively. He has over 20 years of teaching experience at the undergraduate and graduate levels at several educational institutions, as well as 16 years of research experience in applied mathematics. He is a life member of the Indian Society for Technical Education (ISTE), Ramanujan Mathematical Society (RMS), International Association of Engineers (IAENG), and the Indian Society of Structural Engineers (ISSE).

Dr. Hariharan has served as the principal investigator of projects for the DRDO-NRB (Naval Research Board) and Government of India, and has contributed research papers on several interdisciplinary topics such as wavelet methods, mathematical modelling, fractional calculus, enzyme kinetics, ship dynamics, and population dynamics. He has published over 85 peer-reviewed research papers on differential equations and their applications in various leading international journals, including: *Applied Mathematics and Computation*, *Electrochimica Acta*, *Ocean Engineering*, *Journal of Computational and Nonlinear Dynamics*, *MATCH-Communications in Mathematical and Computer Chemistry*, *Aerospace and Space Sciences*, and the *Arabian Journal for Science and Engineering*. In addition, Dr Hariharan serves on the editorial boards of several prominent journals, including: *Communications in Numerical Analysis*, *International Journal of Modern Mathematical Sciences*, *International Journal of Computer Applications*, and *International Journal of Bioinformatics.*

Nomenclature

b	Microbial death constant, cm^3/(mg day)
D_f	Diffusion coefficient within the biofilm, cm^2/day
J	Substrate flux into the biofilm, (mg cm^2)/day
K	Michaelis–Menten constant, mg/cm^3
L_f	Biofilm thickness, cm
q	Substrate consumption rate constant, day^{-1}
S	Dimensionless substrate in the biofilm
S_f	Substrate concentration in the biofilm, mg/cm^3
S_L	Dimensionless substrate concentration outside the biofilm
S_I	Substrate concentration outside the biofilm, mg/cm^3
T	Time, days
x, y	Dimensionless coordinate, cm
X_t	Concentration of physiologically active microorganisms, mg/cm^3

Chapter 1
Reaction–Diffusion (RD) Problems

1.1 Reaction–Diffusion Equations (RDEs)

Reaction–diffusion equations (RDEs) are nonlinear parabolic Partial Differential Equations (PDEs). RDE arises in many applications which include physical sciences, biological sciences, ecology, physiology, finance, to name a few. Reaction–diffusion systems are usually coupled systems (multiple numbers) of parabolic partial differential equations. In population dynamics, the reaction term models growth, and the diffusion term accounts for migration. A few reaction–diffusion (RD) models are models for pattern formation in morphogenesis, for predator–prey and other ecological systems, for conduction in nerves, for epidemics, for carbon monoxide poisoning, and for oscillating chemical reactions.

A simplest form of RDE:

$$u_t = \frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u)$$

where $u = u(x, t)$ is the vector of dependent variables, $f(u)$ is a nonlinear vector-valued function of u (the reaction term), and D is the diffusion coefficient. The reaction term arises from any interaction between the components of u. The parameter u may be a vector of predator–prey interactions, competition, or symbiosis. The diffusion terms may represent molecular diffusion or some 'random' movement of individuals in a population.

A simplest form of reaction–diffusion–convection type is given by

$$\frac{\partial u}{\partial t} = u_t = f(u) + D\frac{\partial^2 u}{\partial x^2} + C\frac{\partial u}{\partial x},$$

where C is the convection coefficient.

The diffusion mechanism model is the movement of many individuals in an environment or media. The particles reside in a region, which we call Ω is open set

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of R^n (the nth-dimensional space with Cartesian coordinate system) with $n \geq 1$. The diffusion coefficient $D(x)$ is not a constant in general since the environment is usually heterogeneous. But when the region is approximately homogeneous, we can assume that $D(x) = D$, the above equation can be simplified to

$$\frac{\partial P}{\partial t} = D\Delta P + f(t,\ x,\ P),$$

where $\Delta P = \mathrm{div}(\nabla P) = \sum_{i=1}^{n} \frac{\partial^2 P}{\partial x_i^2}$ is the Laplacian operator.

In order to develop reaction–diffusion models as dynamical systems, we need to define appropriate state spaces of functions and determine how the models act on them.

1.2 Importance of Reaction–Diffusion (RD) Problems

(i) **Chemical Engineering**: Theoretical models of steady- and unsteady-state reaction–diffusion problems have been developed to obtain the substrate and product concentrations for enzymes immobilized within particles. Reaction–diffusion models are characterized by carbon monoxide poisoning, nitrogen oxide removal, oscillating chemical reactions, pulse splitting and shedding, Rayleigh–Benard convection, and kinetics of methylene blue adsorption (film–pore diffusion model). A theoretical model based on the Michaelis–Menten enzymatic conversion of the substrate and the diffusion of the substrate was created. They also describe the steady-state oxygen diffusion in a spherical cell and equilibrium of isothermal gas sphere, flame propagation, autocatalytic chemical reactions, and neutron population in a nuclear response and branching.

(ii) **Biological and Medical Sciences**: A few important applications of reaction–diffusion equations include population dynamics models, gene propagation models, ecological invasions, a spread of epidemics, tumor growth, and wound healing, distribution of heat sources in a human head, transmission of pulses in nerves, and neurophysiology.

(iii) **Mechanical Engineering**: A simplified kinematical description of a rigidly rotating spiral induced in a general two-component reaction–diffusion medium is elaborated by application of a free-boundary approach. The potential energy generated by an external force as a result of a deformation is propagated among mass points by the principle of reaction and diffusion.

(iv) **Civil Engineering**: A theoretical model based on fundamental reaction–diffusion principles has been formulated to describe the process of concrete carbonation. It is a major time-limiting factor for the durability of reinforced concrete.

1.3 A Few Familiar Reaction–Diffusion Equations (RDEs)

1.3.1 Nonlinear Singular Boundary Value Problem (Lane–Emden Type) and Wavelets

Nonlinear singular boundary value problem (Lane–Emden type) is a significant model in the theory of stellar structure. It models many phenomena in mathematical physics and astrophysics. Most of the work in the stellar structure was initiated by Chandrasekhar [1]. It is a nonlinear differential equation which describes an equilibrium density distribution in the self-gravitating sphere of polytrophic isothermal gas and has a regular singularity at the origin. This model equation was first studied by the astrophysicist Lane [2] who considered the temperature variation of a spherical gas cloud under the mutual attraction of its molecules and subject to the laws of classical thermodynamics. The polytrophic theory of stars was studied by Davis [3]. It primarily deals with the issue of energy transport, through the transfer of material between levels of the star and modeling of clusters of galaxies. Mostly, problems with regard to the diffusion of heat perpendicular to the surfaces of parallel planes are represented by the heat equation. In particular for a polytropic equation of state, the Lane–Emden equation arises.

Due to the simplicity, the wavelets are very effective for solving ordinary differential and partial differential equations [4–9]. Therefore, the idea, to apply wavelet technique also for solving reaction–diffusion problem, arises. The wavelet methods with far less degrees of freedom and with smaller CPU time provide better solutions than classical ones [10–19]. The accuracy and effectiveness of the method are analyzed; the results obtained are compared with the results of other authors (using classical numerical techniques) and with the exact solution, evaluating the error.

1.4 Fractional Differential Equation (FDE)

Fractional calculus is a field of mathematical study that deals with investigations and applications of derivatives and integrals of noninteger orders. In recent years, fractional differential equations have been applied for efficient models in research areas as diverse as dynamical systems, control systems, mechanical systems, chaos, anomalous diffusive and subdiffusive systems, continuous time random walks, wave propagation, and so on.