Numerical Analysis and Simulation of Stiff Reaction-Diffusion Systems and Nonlinear Wave Equations with Damping Effects

Jyoti (20BS0007)
Department of Mathematical Sciences,
Rajiv Gandhi Institute of Petroleum Technology, Jais, Amethi, UP, India

Abstract:

Partial Differential Equations (PDEs) are crucial in modeling various physical phenomena across disciplines such as mathematical biology, environmental engineering, fluid dynamics, and wave propagation in electromagnetics and acoustics. Many problems governed by parabolic and hyperbolic PDEs exhibit complex behaviors, including pattern formation in chemical and biological systems and crack propagation in solid mechanics. Due to the inherent complexity of these equations, analytical solutions are often infeasible, necessitating the use of numerical methods for accurate approximations. A significant challenge in solving these PDEs numerically is stiffness, which arises from interactions between processes occurring at multiple spatial and temporal scales. High-order accurate methods are essential to resolve such problems efficiently. However, classical explicit methods suffer from severe stability constraints when dealing with stiffness, while fully or partially implicit schemes provide better stability but introduce higher computational costs. This trade-off underscores the need for advanced numerical methods that balance stability, accuracy, and computational efficiency while preserving key physical properties.

Chapter 1 presents an introduction and a brief literature review of such PDEs, highlighting the numerical challenges associated with solving stiff systems and the essential physical properties that numerical schemes must satisfy.

Chapter 2 introduces a class of unconditionally strong stability preserving (SSP) multi-derivative methods for the numerical simulation of stiff reaction-diffusion systems. The unconditional SSP property ensures that these methods remain stable without restrictive time-step constraints, making them highly efficient for solving reaction-diffusion problems in the stiff regime. Unlike traditional implicit methods, the proposed approach does not require inversion of the coefficient matrix, significantly reducing computational complexity while maintaining accuracy across a wide range of parameters. The theoretical proof of the SSP property is established, ensuring the efficiency of the method. The accuracy of these methods is evaluated using L^{∞}-error analysis, and comparisons with existing literature demonstrate superior performance, even for larger time steps. Numerical simulations of two-dimensional reaction-diffusion systems, including the Brusselator, Gray-Scott, and Schnakenberg models, pose additional challenges due to higher dimensionality, stiffness in both reaction and diffusion terms, and nonlinear reaction dynamics. The proposed methods effectively handled these complexities, offering an accurate and efficient framework for solving such nonlinear systems.

In Chapter 3, the concept of high-order accurate methods with strong stability properties is extended for convection-diffusion systems. A novel class of computationally explicit multiderivative methods has been developed for the numerical solution of convection-dominated diffusion equations, where the dominance of the convection term introduced significant computational challenges and rendered these problems highly hyperbolic. The proposed methods have been designed to preserve strong stability, ensuring efficient simulation of convection-dominated diffusion equations without imposing restrictive time-step constraints. To enhance accuracy, a fourth-order compact finite difference scheme is employed for spatial discretization. The accuracy of these methods is evaluated using L^2- and L^{∞}-error norms, demonstrating improved performance and a wider stability region compared to existing implicit-explicit (IMEX) methods of the same order. Furthermore, the effectiveness and robustness of the proposed methods are validated through numerical simulations of one- and two-dimensional convection-diffusion equations with varying convection and diffusion coefficients.

In Chapter 4, we have developed an energy-preserving, partially implicit method for the simulation of undamped acoustic and soliton wave propagation in homogeneous and heterogeneous mediums. The derived method is second-order accurate in time and preserves the physical properties of the wave propagation problems. The numerical properties of the methods are evaluated using Fourier analysis for one- and two-dimensional linear wave equations. Energy-preserving properties of the fully discrete scheme are validated through theoretical analysis and numerical experiments. Convergence analysis is also performed to assess the rate of convergence of the developed scheme. Moreover, to assess the efficiency and accuracy of the developed method, several numerical simulations are performed for acoustic wave propagation in two- and three-layered mediums. Simulations of the corner-edge model, nonlinear sine-Gordon, and Klein-Gordon equations in homogeneous and heterogeneous mediums validate the accuracy and efficiency of the developed method.

In Chapter 5, we have extended the concept of energy-preserving space-time discretization methods for damped wave equations. The developed method is implemented with a fourth-order compact finite difference scheme for the numerical simulation of damped linear and nonlinear wave equations. The damped wave equation is an extension of the classical wave equation that includes a damping term to model energy dissipation over time. Theoretical convergence analysis is established, and discrete energy errors for the developed method are computed for wave propagation in the homogeneous and inhomogeneous mediums by considering the relative errors. The theoretical convergence rate is also validated numerically using the discrete L^2- norm. The accuracy of the developed method is validated through various cases of wave and soliton propagation.

In Chapter 6, we summarized our research work, drawn conclusions based on our findings, and provided recommendations for future research directions.

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