Multiscale Simulation and Analysis of Reaction-Diffusion Systems Across Spatial and Temporal Scales

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**Abstract:**

Dynamical systems integrating reaction and diffusion processes often exhibit complexity due to the interplay of phenomena across varying temporal and spatial scales, resulting in reaction-diffusion systems. These systems find applications in disciplines such as pattern formation, mathematical biology, and computational finance. In discrete computations, complexity arises from processes occurring at different scales interacting with each other. Solving such systems numerically requires efficient methods to manage computational costs effectively. Numerical methods that exploit problem structure and identify error sources can significantly optimize simulations by accurately selecting system parameters.

Chapter 1 introduces two-derivative implicit-explicit Runge-Kutta methods for solving physical systems featuring reaction and diffusion terms. These systems include the Allen-Cahn equation modeling phase separation with stiff nonlinearities and the Schnakenberg model for reaction kinetics. Efficient and accurate numerical methods are crucial for parameter variation studies and computational analysis. Explicit methods prove inefficient due to stability and time-step restrictions, leading to the frequent use of implicit methods despite their higher computational cost. The developed methods circumvent the need for matrix inversion, ensuring computational efficiency. Fourier stability analysis validates the methods using two-dimensional scalar reaction-diffusion systems, demonstrating their accuracy in simulating spatiotemporal pattern formations for different models.

In Chapter 2, we have developed a novel implicit-explicit methods for the simulation of the Swift-Hohenberg equation. The Swift-Hohenberg equation is a well-known pattern formation model. The Swift-Hohenberg equation is a fourth-order nonlinear partial differential equation and cannot generally be solved analytically. Stability analysis of the developed method is performed using Fourier analysis for linear Swift-Hohenberg equation. In contrast to the classical implicit-explicit methods, the developed method does not require inversion of the coefficient matrix which minimizes the computational cost. Furthermore, we have also compared stability results with the classical implicit-explicit method for the two-dimensional linear Swift-Hohenberg equation. Moreover, to test the efficiency and robustness of the developed methods we have also performed the simulation of nonlinear Swift-Hohenberg equation.

Chapter 3 deals with the simulation and analysis of liquidity shocks affecting European options in financial markets. A nonlinear reaction-diffusion system governs the mathematical model for liquidity shocks, consisting of coupled differential equations. Implicit-explicit (IMEX) methods are developed to accurately simulate European option pricing, focusing on preserving solution positivity. Consistency and convergence analyses establish theoretical foundations, supported by numerical experiments on uniform and nonuniform meshes, demonstrating the methods' efficiency and accuracy in option pricing under

liquidity shocks. Results indicate first-order convergence for IMEX1 and second-order convergence for IMEX2 methods, offering effective tools for pricing options under liquidity shocks.

In Chapter 4, we investigated the impact of liquidity shocks on option pricing by focusing on American options. Using the methodology developed for European options, which employs a coupled system of differential equations to model liquidity shocks, we have performed simulation and analysis for American options. For numerical analysis, we have utilized implicit-explicit numerical methods to simulate American option pricing under liquidity shocks, ensuring the accuracy and feasibility of solutions while maintaining positivity constraints. Theoretical results for the convergence analysis are established and validated numerically by computing the rate of convergence. Computations are performed on both uniform and nonuniform meshes to validate the accuracy and robustness of the developed methods in capturing the nuanced behavior of American options in the presence of liquidity shocks.

Finally, important conclusions of our research work are outlined in Chapter 5. Future scope of the present work is also discussed in Chapter 5.

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