Numerical Analysis and Simulations of Reactive Dynamical Systems in the Stiff Regime

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Abstract:

Physical systems of interest often exhibit complexity stemming from the interaction of various processes operating at different temporal and spatial scales, resulting in stiff systems of equations that pose significant numerical challenges. Developing efficient numerical methods that exploit the problem structure and sources of stiffness requires diligent effort and care, enabling cost-effective simulations in relevant parameter regimes. While implicit-explicit and fully implicit methods are popular solutions for handling stiff systems by taking larger time steps and solving nonlinear equations, they may require the use of complex linear algebra solvers and result in high computational costs. Hence, there is a need to explore alternative time integration methods that do not rely on linear algebra solvers and minimize computational complexity and CPU time.

Chapter 1 presents a novel class of computationally explicit Runge-Kutta methods that can effectively solve stiff convection-diffusion equations. Unlike traditional implicit methods, the developed methods do not require the inversion of a coefficient matrix, making it computationally efficient. The numerical properties of the methods were evaluated using Fourier stability analysis for a model stiff convection-diffusion equation. The accuracy and efficiency of the developed methods were further assessed by solving compressible Navier-Stokes equation for benchmark problems in computational aeroacoustics, such as laminar flow over stationary and rotationally oscillating cylinders and a NACA0012 airfoil. The computed results were compared with previous direct numerical simulation studies and experimental data, and they demonstrated good agreement. To evaluate the performance of the developed methods, numerical simulations using the classical four-stage Runge-Kutta method were also carried out. The present methods were found to be competitive with the classical Rune-Kutta and low dispersion and dissipation Runge-Kutta methods in terms of numerical accuracy while being more computationally efficient. Spatial derivatives are discretized using compact schemes. The developed methods also effectively captured flow details related to three-dimensional supersonic flow past a sphere. Therefore, the developed methods offer promising time-integration schemes for analyzing unsteady problems governed by stiff systems with better computational performance.

In Chapter 2, we built upon the concepts established in Chapter 1 and created a novel class of computationally explicit Runge-Kutta methods for nonlinear reaction-diffusion systems, which address stiffness in both the reaction and diffusion terms. These methods don't require matrix inversions and as a result, have low computational costs. The methods' accuracy and efficiency are assessed using Fourier analysis and discrete maximum absolute errors for a linear reaction-diffusion model equation, and excellent agreement with exact solutions is obtained. To demonstrate the methods' applicability, we simulated a range of nonlinear stiff reaction-diffusion systems, including phase separation governed by the Allen-Cahn equation, the Schnakenberg model for reaction kinetics, and predicting the morphology of electrodeposition at the interface. We compared our numerical results with those from computational and experimental studies in the literature and found good agreement. These findings show that the proposed methods are valid and effective for simulating a broad range of complex reaction-diffusion systems, and they offer computational efficiency and accuracy superior to traditional methods.

Chapter 3 builds on the concepts introduced in Chapters 1 and 2 to develop time-marching techniques for solving systems of stiff convection-diffusion-reaction equations (CDREs). Fourier analysis is used to evaluate the stability properties of the methods for both one-dimensional and

two-dimensional CDREs, and appropriate values for the free parameters are identified to eliminate the unstable region associated with the explicit Runge-Kutta method. The accuracy and efficiency of the methods are demonstrated by solving various one-dimensional unsteady inhomogeneous CDREs with different grid Fourier and reaction numbers. The results obtained show excellent agreement with the exact solutions, even for high values of grid Fourier number (F_o). The effectiveness of the methods is further demonstrated by solving the contaminant transport model with kinetic Langmuir sorption, with the computed solution matching the exact solution available in the literature. Finally, the accuracy of the developed methods is demonstrated by simulating pattern formations in the two-dimensional chemotaxis model with nonlinear diffusion and volume-filling effect, for both single and double eigenvalues. The solutions obtained are compared with analytic stationary solutions obtained via weakly nonlinear analysis, and excellent agreement is observed in terms of L^2 and H^1 norms of the error.

In Chapter 4, we have introduced a novel family of two-derivative computationally explicit Runge-Kutta-Nyström type time-marching methods to simulate stiff wave equations. Compared to the Runge-Kutta-Nyström method, our two-derivative methods require only two stages to achieve the desired accuracy, resulting in a reduced computational cost. Importantly, the methods do not require inverting the discretized system of algebraic equations. Fourier stability analysis has been used to verify the accuracy of the methods for the one-dimensional bi-directional wave equation model. To demonstrate the robustness and efficiency of the two-derivative methods, we have performed numerical simulations of acoustic wave propagation in heterogeneous media consisting of two and three layers. Additionally, the accuracy of the two-derivative methods has been validated by numerically simulating the damped and undamped cases of the sine-Gordon equation with various soliton scenarios. The L^∞ and root mean square errors of the two-derivative methods have been compared to those reported in the literature, and our results exhibit excellent agreement with the soliton behavior. Moreover, while dealing with stiff differential equations, it is vital to have accurate and efficient spatial discretization because these equations often involve rapidly varying functions that require high resolution in specific regions of the domain. As a result, we formulated higher-order compact schemes on nonuniform grids to address this issue. The validity of the developed methods was verified through simulations of shallow water and Navier-Stokes equations, demonstrating promising results for the simulations of flow and wave-propagation problems.

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