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On the Stability and CPU Time of the Implicit Runge-Kutta Schemes for Steady State Simulations

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Abstract. Implicit time integration schemes are popular because their relaxed stability constraints can result in better computational efficiency. For time-accurate unsteady simulations, it has been well recognized that the inherent dispersion and dissipation errors of implicit Runge-Kutta schemes will reduce the computational accuracy for large time steps. Yet for steady state simulations using the time-dependent governing equations, these errors are often overlooked because the intermediate solutions are of less interest. Based on the model equation $dy/dt=(\mu+i\lambda)y$ of scalar convection diffusion systems, this study examines the stability limits, dispersion and dissipation errors of four diagonally implicit Runge-Kutta-type schemes on the complex $(\mu+i\lambda)\Delta t$ plane. Through numerical experiments, it is shown that, as the time steps increase, the A-stable implicit schemes may not always have reduced CPU time and the computations may not always remain stable, due to the inherent dispersion and dissipation errors of the implicit Runge-Kutta schemes. The dissipation errors may decelerate the convergence rate, and the dispersion errors may cause large oscillations of the numerical solutions. These errors, especially those of high wavenumber components, grow at large time steps. They lead to difficulty in the convergence of the numerical computations, and result in increasing CPU time or even unstable computations as the time step increases. It is concluded that an optimal implicit time integration scheme for steady state simulations should have high dissipation and low dispersion.

AMS subject classifications: 65M22, 65M12, 76M20, 76M25

Key words: Runge-Kutta, implicit time integration, dispersion, dissipation, numerical stability, steady state simulation.

1 Introduction

In engineering applications, steady state solutions (viewed as the long-time mean of the unsteady solutions, or the final state of diffusion systems) are frequently sought at the

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design stage, since the solutions are relative inexpensive and can reveal well the performance of the systems. Practical numerical simulations are marched in time to steady state solutions, because the hyperbolic nature of the time-dependent equations facilitates the boundary treatments and the solutions of the discretized, explicit or implicit equation systems. Quasi-steady state solutions are obtained as the time derivatives diminish to machine zero at large time.

The semi-discretized form of the governing equations corresponds to the first-order ordinary differential equation (ODE) with the initial condition:

$$\frac{dQ}{dt}=R(t,Q), \qquad Q(t_0)=Q^0, \tag{1.1}$$

where R denotes the residuals that consist of spatial derivatives of the dependent variables. Numerous time integration schemes have been developed to acquire the numerical solutions at discrete time steps, such as the Crank-Nicolson scheme [1], the Lax-Wendroff scheme [2], the Taylor-Galerkin scheme [3] and the multi-stage Runge-Kutta schemes [4]. Of particular interest in this study are the implicit Runge-Kutta schemes. Some traditional schemes, such as the Crank-Nicolson scheme, can be cast into the form of Runge-Kutta schemes as well.

For time-accurate simulations, development has been mainly focused on high-order, A-stable schemes. Because the leading error term of the order n is proportional to Δt^n, a high-order scheme with a relaxed stability limit permits larger time steps to improve the computational efficiency, given the same requirement of the computational accuracy [5,6]. However, for more sensitive nonlinear wave propagation phenomena, studies in the past two decades have shown that much smaller time steps than those allowed by the stability limits are necessary to minimize the numerical errors in the amplitude (dissipation errors) and the phase (dispersion errors) of all wave components of interest. Therefore, optimized high-order, low-dissipation and low-dispersion time advancement schemes have been proposed for nonlinear wave propagation simulations [7–13].

For quasi-steady solutions, design of unconditionally stable schemes has been the main objective in the past research. The order of accuracy in time and the dispersion and dispersion errors are of minor concerns since the intermediate solutions are of no interest. In fact, excessive dissipation is preferred to accelerate the convergence of low wavenumber error components, and this is the basis of the convergence acceleration techniques such as implicit residual smoothing [14,15].

However, applications show that some A-stable schemes may still become unstable for large time steps, although the A-stable property suggests that numerical errors will decay or remain bounded for arbitrary time steps, [6,16]. Unstable computations appear when the large oscillations of the numerical solutions overwhelm the physical solutions. Some remedies have been proposed, such as the S-stable schemes [17], the total variation diminishing (TVD) [18] and strong stability-preserving (SSP) [19–22] time discretization.

In addition, implicit time integration schemes serve to improve the computational efficiency by allowing the largest possible time steps to advance the time-dependent solu-