Applied Mathematics and Computation 304 (2017) 41–57

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Global spectral analysis of multi-level time integration schemes: Numerical properties for error analysis

Tapan K. Sengupta[a,*], Aditi Sengupta[b], Kumar Saurabh[a]

[a] High Performance Computing Laboratory, Department of Aerospace Engineering, I. I. T. Kanpur, Kanpur 208016, India
[b] Ph.D. candidate, Dept. of Engg., Univ. of Cambridge, UK.

ARTICLE INFO

Keywords:
Three-time level integration method
Global spectral analysis
Spurious mode
Adams–Bashforth method
Absolute instability
Effects of filtering

ABSTRACT

An analysis is reported here for three-time level integration methods following the global spectral analysis (GSA) described in *High Accuracy Computing Methods*, T.K. Sengupta, Cambridge Univ. Press, USA. The focus is on the second order Adams–Bashforth (AB2) and the extrapolation in time (EXT2) methods. Careful distinction is made for the first time step at $t = 0$ by either Euler forward or four-stage, fourth order Runge–Kutta (RK4) time schemes. The latter is used to solve a benchmark aeroacoustic problem. Several one-dimensional wave propagation models are analyzed: pure advection and advection-diffusion equations. Various spatial discretizations are discussed, including Fourier spectral method. Attention is paid to the presence of physical and numerical modes as noted in the quadratic equation obtained from the difference equation for the model 1D convection equation. It is shown that AB2 method is less stable and accurate than EXT2 method, with respect to numerical dissipation and dispersion. This is true for the methods, in which the physical mode dominates over the numerical mode. Presented analysis provides useful guide to analyze any three-time level methods.

1. Introduction

In simulating fluid flow and wave phenomena, less attention is paid to study time discretization in depth, except those in [31,33,38,40]. It is well known that the order of time derivative present in the governing equation should be equal to that of numerical amplification factor, e.g., a governing equation with first time derivative should have only one numerical amplification factor, for the physical mode in the continuum, and this is achieved by two-time level methods. Taking first order, forward Euler time stepping method turns out to be numerically unstable and for this reason use of four-stage two-time level Runge–Kutta (RK4) schemes [31] are used for higher accuracy. For example, optimal three- and four-stage, time integration methods along with compact schemes for spatial discretization have been proposed in *OCRK*3 and *ORK*4 methods, which ensures dispersion relation preservation (DRP) properties [2,36].

One analyzes one-dimensional convection equation [28,31,34] in the context of evaluating space-time discretization together to quantify the main sources of numerical errors. For this, the model equation in Cauchy framework is,

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}; \quad \text{for } c > 0, \quad -\infty \le x \le +\infty \tag{1}$$

* Corresponding author.
E-mail addresses: tksen@iitk.ac.in, tapansg@gmail.com (T.K. Sengupta).

http://dx.doi.org/10.1016/j.amc.2017.01.026
0096-3003/

The motivation for using this governing equation in an infinite domain is that one does not require any boundary condition and the initial condition is propagated to the right. Reflections or influence from the boundaries are avoided also. Thus, devoid of any need for using boundary condition, gives one an impression that one can study this model equation in a local framework. It is noted by Vichnevetsky [46] that the spirit of this assumption is identical to that used in the standard von Neumann method of analysis of numerical stability [24], in which local modes of instability are mathematically described as holding every where, and in the present exposition we provide instead a global analysis (also known as global spectral analysis or GSA). This GSA method involves estimation of effects of both space and time discretizations considered together and is described next. One of the desirable features of GSA is that this is not restricted to periodic problem, unlike von Neumann Fourier analysis.

For the GSA of numerical schemes, let us represent the unknown in the hybrid spectral plane (with time in physical plane and space in wavenumber (k) plane, with ranges defined by the Nyquist limit, $k_{max} = \pi/h$), given by,

$$u(x,t) = \int_{-k_{max}}^{k_{max}} U(k,t)e^{ikx}dk \tag{2}$$

In the continuum limit, $h \to 0$, the limits of the integrand will extend to infinity. Upon spatial discretization in a finite domain with h as the uniform grid spacing, one would be working within the Nyquist limit. An exact spatial discretization of $u(x, t)$ can be obtained as,

$$\left.\frac{\partial u}{\partial x}\right|_{exact} = \int ikU(k,t)e^{ikx}dk \tag{3}$$

with integral extending from $-\infty$ to $+\infty$. In a similar way, the numerically evaluated spatial derivative is expressed as [31],

$$\left.\frac{\partial u}{\partial x}\right|_{num} = \int_{-k_{max}}^{k_{max}} ik_{eq}U(k,t)e^{ikx}dk \tag{4}$$

In [26,31], the expressions for k_{eq} have been reported for a large number of spatial discretization by explicit and implicit methods. In most analyses of numerical methods, however, only spatial discretization is only considered, as in [26,44]. Additionally, most of these analyses [26,28,44–48] were performed for an interior point in isolation (as noted in [46] above). One of the early developments in GSA is the introduction of analyzing spatial discretization globally for the full domain [35], as a distinct necessity for implicit spatial discretization. GSA was introduced to overcome this gap in the existing methods to calibrate numerical schemes by following the correct numerical dispersion of Eq. (1). The major finding of this aspect of GSA is that computationally the constant phase in Eq. (1), does not remain a constant. Instead the numerical phase speed (c_N) is found to be a function of wavenumber (k), an attribute causing dispersion of numerical solution. For Eq. (1), the exact dispersion relation is given by,

$$\omega = kc. \tag{5}$$

In [17,31,33,34], the numerical dispersion relation has been derived as,

$$\omega_N = kc_N. \tag{6}$$

In contrast to Eq. (6), authors in [45,46] and in many other references have taken the numerical dispersion relation to be of the form,

$$\omega_N = k_{eq}c \tag{7}$$

where k_{eq} is as given by Eq. (4), originating from spatial discretization alone. This is an assumption based on the fact that the prescribed phase speed (c) remains constant during numerical integration. Also, taking the numerical wavenumber as the equivalent wavenumber for spatial discretization is adopted without rigorous proof. If spatial discretization decides k_{eq}, then why shouldn't one choose ω_N corresponding to temporal discretization? These queries are not addressed in framing Eq. (7). In contrast, Eq. (6) is directly obtained by performing spatial and temporal discretization of the governing differential equation. This brings us to the very important observation that even when one is solving a constant coefficient equation (such as Eq. (1) [34] or the heat equation [32]) has shown that the coefficient in the governing equation becomes function of wave number. Such uncertainty is inherent with scientific computing and this was lost in von Neumann analysis, by adopting Eq. (7), instead of Eq. (6). In the following, we show the consequence of adopting GSA as opposed to following von Neumann analysis for error dynamics.

By definition, in many physical situations (as in Eq. (1)) dispersion relation is another form of governing differential equation in physical plane, expressed in the spectral plane. The dispersion relation in Eq (7) does not take into the effect of temporal discretization and thus lacks fundamentally as an analysis tool. In contrast, the numerical dispersion in Eq. (6) is obtained from the simultaneous discretization in space and time for the governing equation. We just note that in some physical situations, dispersion relation relates space and time scales of the problem arising from the boundary condition. At present, Eq. (1), expressed as the Cauchy problem does not even require boundary condition to characterize it.

For Eq. (1) the wrong dispersion relation (Eq. (7)) is a consequence of the implicit assumption in von Neumann error and stability analysis, which assumes that the numerical solution and corresponding error as function of space and time, $e(x, t)$,