Journal of Computational Physics 228 (2009) 4182–4199

Contents lists available at ScienceDirect

Journal of Computational Physics

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

A general strategy for the optimization of Runge–Kutta schemes for wave propagation phenomena

Matteo Bernardini, Sergio Pirozzoli *

Università degli Studi di Roma "La Sapienza", Dipartimento di Meccanica e Aeronautica, Via Eudossiana 18, 00184 Roma, Italy

ARTICLE INFO

Article history:
Received 8 September 2008
Received in revised form 17 February 2009
Accepted 19 February 2009
Available online 6 March 2009

Keywords:
Computational aeroacoustics
Runge–Kutta schemes
Optimized algorithms
Numerical dispersion
Numerical dissipation

ABSTRACT

We analyze optimized explicit Runge–Kutta schemes (RK) for computational aeroacoustics, and wave propagation phenomena in general. Exploiting the analysis developed in [S. Pirozzoli, Performance analysis and optimization of finite-difference schemes for wave propagation problems, J. Comput. Phys. 222 (2007) 809–831], we rigorously evaluate the performance of several time integration schemes in terms of appropriate error and cost metrics, and provide a general strategy to design Runge–Kutta methods tailored for specific applications. We present families of optimized second- and third-order Runge–Kutta schemes with up to seven stages, and describe their implementation in the framework of Williamson's 2*N*-storage formulation [J.H. Williamson, Low-storage Runge–Kutta schemes, J. Comput. Phys. 35 (1980) 48–56]. Numerical simulations of the 1D linear advection equation and of the 2D linearized Euler equations are performed to demonstrate the validity of the theory and to quantify the improvement provided by optimized schemes.

1. Introduction

In the past decades intense efforts in computational aeroacoustics (CAA) have been devoted to develop schemes with minimal numerical dissipation and dispersion. Ideal CAA schemes should be able to propagate over long distances and for long times acoustic disturbances with a broad range of length and time scales. High order schemes for CAA are generally based on a method-of-lines approach, whereby spatial and time discretization are handled sequentially. Most of the efforts have been directed on trying to improve the discretization of the space derivative operators. For this purpose Lele [3] proposed central compact schemes, which guarantee resolution properties in wavenumber space similar to spectral ones. Central approximations of the spatial derivatives have null dissipation error, and this is the reason for their superiority in CAA with respect to upwind schemes. The basic idea of compact schemes is to improve the resolution properties of derivative approximations by minimizing the difference between the exact and the discrete dispersion relation. A wide variety of "optimized" schemes for spatial discretization are available in the literature [3–6], with varying degree of success, but mostly based on the attempt to give up maximum formal order of accuracy in the representation of the derivatives while improving the behavior in wavenumber space.

The issue of time integration of the semi-discretized set of ordinary differential equations (ODE) associated with a given spatial discretization has received comparatively less attention. Time integration in CAA applications is usually performed by means of classical, explicit third- or fourth-order Runge–Kutta algorithms [7], because of their simplicity of implementation and relatively large stability limits. Given a general non-autonomous system of ODEs stemming from the semi-discretization of a conservation law, symbolically written as

* Corresponding author. Tel.: +39 06 44585202; fax: +39 06 4881759.
E-mail addresses: matteo.bernardini@uniroma1.it (M. Bernardini), sergio.pirozzoli@uniroma1.it (S. Pirozzoli).

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2009.02.032

$$\frac{d\mathbf{U}}{dt} = \mathbf{F}(\mathbf{U}(t), t), \tag{1}$$

where $\mathbf{U}$ is the vector of point unknowns at time t, the general form of an explicit s-stage, two-level RK scheme to advance from time t^n to $t^n + k$ is

$$\mathbf{U}^{n+1} = \mathbf{U}^n + k\sum_{i=1}^{s} b_i\mathbf{K}_i, \tag{2a}$$

$$\mathbf{K}_i = \mathbf{F}\left(\mathbf{U}^n + k\sum_{j=1}^{i-1} a_{ij}\mathbf{K}_j, t^n + kc_i\right), \quad i = 1, \ldots, s, \tag{2b}$$

with

$$c_i = \sum_{j=1}^{i-1} a_{ij}. \tag{3}$$

The coefficients a_{ij} and b_i can be determined in such a way as to achieve a given formal order of accuracy and/or to improve the computational efficiency. For example, to derive RK schemes with up to third-order of accuracy, the following conditions [7] must be satisfied

$$(O1): \quad \sum_{i=1}^{s} b_i = 1, \tag{4a}$$

$$(O2): \quad \sum_{i=1}^{s} b_i c_i = \frac{1}{2}, \tag{4b}$$

$$(O3): \quad \sum_{i=1}^{s} b_i a_{ij} c_j = \frac{1}{6}, \tag{4c}$$

$$(O4): \quad \sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3}, \tag{4d}$$

where (On) indicates formulas controlling nth-order of accuracy.

A few attempts have been made to improve the performance of RK schemes, with the broad idea of minimizing the incurred dispersion and dissipation error. Hu et al. [8] introduced a class of Low-Dissipation and Dispersion Runge–Kutta (LDDRK) schemes by minimizing (a suitable norm of) the difference between the amplification factor of the RK scheme and the "true" amplification factor. Those authors considered (linearly) second-order accurate schemes with four and five stages and fourth-order accurate ones with six stages, and 3N-storage implementation (i.e. requiring memory allocation proportional to three times the number of ODEs to be solved). For nonlinear problems the accuracy of the schemes proposed by Hu et al. drops to second-order.

Low-storage implementation is an important issue in CAA because of the extensive computational resources required by wave propagation problems in large domains. Kennedy et al. [9] have derived low-storage, explicit Runge–Kutta schemes, that use from two to five registers of memory, and having accuracy from third- to fifth-order. Those authors optimized schemes across a broad range of properties, such as linear and nonlinear stability, accuracy efficiency, error control reliability, dissipation and dispersion errors.

Stanescu and Habashi [10] devised 2N-storage implementations of many RK schemes, which maintain the formal order of accuracy also for nonlinear operators, by exploiting Williamson's [2] formulation, and enforcing constraints deriving from order of accuracy, storage and resolution requirements. In particular, they provided a low-storage implementation of LDDRK schemes developed by Hu et al. [8].

An alternative low-storage implementation was introduced by Calvo et al. [11], who proposed optimized third- and fourth-order, five-stage schemes. Their optimization strategy is based on first maximizing the stability range of the algorithm, and then trying to improve the range of well-resolved Courant numbers. The same authors [12] also proposed a variant of the method whereby the coefficients of the scheme were determined so as to maximize the sum of the stability and the accuracy range.

Bogey and Bailly [13] developed optimized second-order, five- and six-stage RK schemes based on minimizing the sum of the norms of the dissipation and dispersion errors in a given range of frequencies. Their strategy was also used by Berland et al. [14] to derive an optimized fourth-order accurate (in nonlinear sense) low-storage RK algorithm with a wide stability range.

Ramboer et al. [15] brought spatial discretization into the analysis, and attempted to minimize the total dissipation and dispersion errors deriving from coupling with time integration. The formulation of Ramboer et al. has the main advantage of being applicable also to upwind type schemes, as opposed to conventional strategies based on the assumption of central spatial discretizations.