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On some new low storage implementations of time advancing Runge–Kutta methods☆

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In this paper, explicit Runge–Kutta (RK) schemes with minimum storage requirements for systems with very large dimension that arise in the spatial discretization of some partial differential equations are considered. A complete study of all four stage fourth-order schemes of the minimum storage families of Williamson (1980) [2], van der Houwen (1977) [8] and Ketcheson (2010) [12] that require only two storage locations per variable is carried out. It is found that, whereas there exist no schemes of this type in the Williamson and van der Houwen families, there are two isolated schemes and a one parameter family of fourth-order schemes in four stage Ketcheson's family. This available parameter is used to obtain the optimal scheme taking into account the $\| \cdot \|_2$ norm of the coefficients of the leading error term. In addition a new alternative minimum storage family to the s-stage Ketcheson that depends also on $3s - 3$ free parameters is proposed. This family contains both the Williamson and van der Houwen schemes but it is not included in Ketcheson's family. Finally, the results of some numerical experiments are presented to show the behavior of fourth-order optimal schemes for some nonlinear problems.

1. Introduction

This paper deals with the numerical solution of IVPs for systems of ordinary differential equations

$$\frac{\mathrm{d}}{\mathrm{d}t} u(t) = f(u(t)), \qquad u(t_0) = u^0 \in \mathbf{R}^N, \tag{1}$$

where the dimension N is assumed to be large, by means of explicit Runge–Kutta (RK) methods. For simplicity, we will consider only autonomous systems although the results easily extend to nonautonomous systems.

In standard explicit s-stage RK methods [1], the numerical solution u^n of (1) at the time level t_n is advanced to the next time level $t_{n+1} = t_n + \Delta t$ by means of the algorithm

$$u^{n+1} = u^n + \Delta t \sum_{j=1}^{s} b_j f(Y_j), \tag{2}$$

$$Y_j = u^n + \Delta t \sum_{i=1}^{j-1} a_{ji} f(Y_i), \quad (j = 1, \ldots, s), \tag{3}$$

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where the stages $Y_j \in \mathbf{R}^N,\ j = 1, \dots, s$ are computed successively from (3) with s function evaluations and then by means of (2) we get the new approximation u^{n+1}. Here $b = (b_i)$, $A = (a_{ij})$, $1 \le j < i \le s$ are the $s + s(s-1)/2 = s(s+1)/2$ real parameters that define the method and can be written in the $(s+1) \times (s+1)$ lower triangular Butcher array

$$\widehat{A} = (a_{ij})_{i,j=1,\dots,s+1} = \left(\begin{array}{c|c} A & 0^T \\ \hline b^T & 0 \end{array}\right) \equiv \begin{pmatrix} 0 & & & & \\ a_{21} & 0 & & & \\ a_{31} & a_{32} & 0 & & \\ \vdots & & & \ddots & \\ b_1 & b_2 & \cdots & b_s & 0 \end{pmatrix}. \tag{4}$$

Observe that introducing the vector notations

$$Y = (Y_j)_{j=1}^{s+1} \in (\mathbf{R}^N)^{s+1}, \quad \text{with } Y_{s+1} = u^{n+1}, \qquad f(Y) = (f(Y_j))_{j=1}^{s+1},$$

and $e = (1, \dots, 1)^T \in \mathbf{R}^{s+1}$ the Eqs. (2), (3) can be written as

$$Y = \Delta t(\widehat{A} \otimes I_N) f(Y) + e \otimes u^n. \tag{5}$$

In usual applications the free parameters of $\widehat{A}$ are selected taking into account different stability and accuracy (local-, dispersion- and dissipation-errors) requirements that depend on the class of problems (1) to be integrated. The implementation of (2), (3) requires in general the use of $s+1$ registers of size N to complete each step and there are time advancing problems which arise in the semidiscretization of some PDEs in which N is very large. This fact implies that the efficiency of the RK method depends strongly on the number of registers used in the computation and therefore methods with minimum storage requirements are preferred. Thus, for a given number of stages s, we want to consider minimum storage methods, i.e. that can be implemented with two N-registers, having the best stability and accuracy properties.

The simplest minimum storage one-step method is Euler's method that requires only two N-registers and consequently the simplest s-stage minimum storage method results of a repeated application of Euler's method with step sizes $c_j\Delta t,\ j = 1, \dots, s$ with $\sum_{j=1}^{s} c_j = 1$, however their accuracy is not enough in many applications. Within the minimum storage schemes (two registers of size N), the $(2N)$-schemes of Williamson [2] have been very popular in Computational Aeroacoustics (CAA) problems in the last years. Thus Stanescu and Habashi [3] have derived several $(2N)$-schemes with amplification functions obtained in [4] that minimize the dissipation and dispersion errors for the linear wave test equation. Other fourth-order (nonlinear) $(2N)$-schemes with minimum local error were derived in [5]. More recently $(2N)$-storage schemes addressed to problems in the field of computational aeroacoustic have been proposed in [6,7]. The advantage of Williamson schemes over Euler's compositions is that s-stage Williamson methods have $2s-1$ free parameters and then allow us to obtain better accuracy and stability properties than in s-stage Euler's compositions.

Alternative families of minimum storage schemes, proposed in ([8] Eq. (2.2.4)′) and referred to as $(2R)$-schemes, have been considered also to derive different low storage methods. They have been extensively studied in [9] to obtain optimal schemes of several orders having in mind the semidiscretization of Navier–Stokes equations including also local error control by embedded pairs (of course with additional storage requirements). Also the authors of the present paper [10,11] have obtained some optimal $(2R)$-methods for acoustic problems. It must be noticed that the s-stage $(2R)$-schemes have also $2s-1$ free parameters and therefore have the same flexibility than the Williamson methods, although it can be seen that the $(2R)$- and $(2N)$-families do not contain the same RK methods.

More recently Ketcheson [12] has derived a new family of s-stage minimum storage RK schemes, referred to as $(2S)$-schemes, with $3s-3$ free parameters that does not contain all s-stage $(2N)$- and $(2R)$-schemes but possess a greater flexibility than the above two families. This author has employed these schemes in [13] to obtain optimal strong stability preserving methods for hyperbolic conservation laws. Further he has found [12] several four stage $(2S)$-schemes with order four. Observe that the class of four stage RK methods depends on 10 parameters and there are 8 (non linear) conditions for order four. Since in the $(2S)$-schemes with $s = 4$ there are $3s - 3 = 9$ free parameters, one expects in principle to have a one dimensional family of fourth-order methods. On the other hand, for the $(2N)$- and $(2R)$-schemes with $s = 4$, the number of available parameters is $2s - 1 = 7$ and we cannot in general to satisfy the 8 nonlinear conditions for order four. However, for the $(2N)$-schemes, Williamson has shown in [2] that there exist special $(2N)$-schemes where some coefficients tend to zero while others tend to infinity that attains order four when applied to special differential systems with vector fields $f(y)$ that remain bounded when $|y| \to \infty$.

The aim of this paper is two fold: First of all we want to identify the four stage RK methods with order four that can be written as $(2S)$-schemes for general vector fields. It will be found that there are a one parameter family of four stage $(2S)$-schemes with order four together with another two isolated schemes. An optimal scheme of this family is selected in the sense that minimizes the Euclidean norm of the coefficients of the leading error terms. Secondly, a new family of minimum storage RK schemes that depends on $3s-3$ parameters and extends naturally the $(2N)$- and $(2R)$-families is proposed. Moreover, the relation with the $(2S)$-schemes of Ketcheson is studied.