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NOTE

2*N*-Storage Low Dissipation and Dispersion Runge-Kutta Schemes for Computational Acoustics

1. INTRODUCTION

For physical problems that involve accurate time-dependent wave propagation, as those arising in acoustics, the usual requirement of a high-order truncation error does not guarantee that a numerical method yields accurate results. Indeed, as has been pointed out mainly in [1], the dissipation and dispersion properties of the numerical method are very important for computing wave solutions of systems of partial differential equations. This is valid for both the spatial and the time discretization methods. The explicit Runge-Kutta (RK) methods are widely used to discretize the time derivative because of their advantages that include flexibility, large stability limits, and ease of programming. Hu and co-workers [2] showed that the dissipation and dispersion properties of the RK methods depend on their coefficients and optimized them for the convective wave equation, obtaining what they called low-dissipation and dispersion Runge-Kutta (LDDRK) methods. These methods are more efficient than classical ones, in terms of work required for a given accuracy, for wave propagation problems.

For large size physical problems, memory requirements may become exhaustive. They can be decreased using special RK schemes that can be written such that only $2N$-storage is required, where N is the number of degrees of freedom of the system (i.e., number of grid points $\times$ number of variables). To design such RK schemes, enough free coefficients must exist such that additional conditions hold between them. Williamson [3] first showed that all second-order and some third-order methods can be written in $2N$-storage form. He also showed that fourth-order four-stage methods cannot be written in this way. By allowing additional stages and using the resulting new free coefficients to impose the $2N$-storage constraints, Carpenter and Kennedy [4] devised a fourth-order, five-stages RK method that is compatible with the classical fourth-order method which however requires at least $3N$ storage.

Hu *et al*. [2] provide $3N$-storage implementations of the LDDRK schemes. These are valid for linear problems only, in the sense that they turn to second order accuracy when applied to nonlinear problems. Since most LDDRK schemes have a number of stages that

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exceeds their order of accuracy, they can in principle be written in $2N$-storage format. The goal of this paper is to devise such implementations. The methods presented here are valid for nonlinear problems, since the explicit imposition of the order conditions guarantees their formal order of accuracy in the general nonlinear case. They do not, however, provide means for monitoring the error since this introduces additional constraints and hence might require additional stages. The required conditions for the coefficients, arising from the order of accuracy, low-storage and low-dissipation/dispersion constraints are developed. They lead to nonlinear systems of equations that are solved numerically. For each scheme a full set of coefficients is provided, chosen among the multiple solutions available. Several numerical results obtained with the proposed and other available RK methods end the paper.

2. GENERAL THEORY

Since wave-propagation problems normally have time-dependent boundary conditions, we consider the general case of a non-autonomous system of ordinary differential equations of the form

$$\frac{dU}{dt} = F(t, U(t)); \qquad U(t_0) = U_0 \tag{1}$$

The general form of an explicit, pth order of accuracy s-stages RK method for computing the numerical approximation u^n to $U(t^n = t^{n-1} + h)$ is

$$\begin{aligned} u^n &= u^{n-1} + h \sum_{i=1}^{s} b_i k_i \\ k_i &= F\left(t^{n-1} + hc_i, u^{n-1} + h \sum_{j=1}^{i-1} a_{ij} k_j \right), \end{aligned} \tag{2}$$

where $c_i = \sum_{j=1}^{i-1} a_{ij}$, $i = 1 \ldots s$.

For the scheme in Eq. (2) to have the required order of accuracy, the coefficients must obey certain order conditions [5]. These are obtained by equating coefficients of the Taylor series development of U. The explicit form of these conditions up to fourth order of accuracy is

$$\begin{aligned} &(O1) \sum b_i = 1, && (O4) \sum b_i c_i^3 = \frac{1}{4} \\ &(O2) \sum b_i c_i = \frac{1}{2}, && (O4) \sum b_i c_i a_{ij} c_j = \frac{1}{8} \\ &(O3) \sum b_i c_i^2 = \frac{1}{3}, && (O4) \sum b_i a_{ij} c_j^2 = \frac{1}{12} \\ &(O3) \sum b_i a_{ij} c_j = \frac{1}{6}, && (O4) \sum b_i a_{ij} a_{jk} c_k = \frac{1}{24}. \end{aligned} \tag{3}$$

In these relations sums on all indices extend from 1 to s; on the left side of each condition we have indicated the order of accuracy that it governs.

To obtain low-storage schemes, the idea is to leave useful information in the storage locations, by writing each successive stage on the same register without zeroing the previously held values. The algorithm becomes (with w/h an approximation to dU/dt),

$$\left.\begin{aligned} w_i &= \alpha_i w_{i-1} + hF(t_{i-1}, u_{i-1}) \\ u_i &= u_{i-1} + \beta_i w_i \end{aligned}\right\}, \qquad i = 1, \ldots, s \tag{4}$$

with $\alpha_1 = 0$ for the algorithm to be self-starting. Here $u_0 = u^{n-1}$, $u^n = u_s$, and $t_i = t^{n-1} + hc_i$. Since only the w and u values must be stored for each degree of freedom, this results in a $2N$-storage algorithm.

Using Eqs. (2) and (4), one can express the usual RK coefficients a_{ij}, b_i in terms of α_i, β_i. Since these relations depend on the number of stages s, they will be presented in detail in the next sections. One can then, in principle, solve the order conditions in terms of the $2N$-storage constants, and obtain valid low-storage RK schemes. For $p = 3, s = 3$ (classical 3rd order RK schemes), it can be seen that there are 5 such constants ($\alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3$) and four order conditions to be satisfied. It seems hence plausible, and this has been confirmed by Williamson [3], that such schemes exist. For $p = 4, s = 4$ there are eight order conditions and only seven free coefficients, and as has also been shown in [3], there are no such schemes.

The dissipation/dispersion and stability properties of the RK methods are closely related, hence they will be discussed together. To this end, we consider the model equation $dU/dt = qU$, $U(0) = 1$, with q a possibly complex constant [5]. Using Eq. (2), it can be found that the amplification factor of a RK method is given by

$$r(z) = \frac{u^n}{u^{n-1}} = 1 + zb^T(I + zA + z^2A^2 + \cdots + z^{s-1}A^{s-1})E, \tag{5}$$

where $z = qh$, $A = [a_{ij}]$ with $a_{ij} = 0$ for $j \geq i$, $b = [b_1, b_2, \ldots, b_s]^T$, and $E = [1, 1, \ldots, 1]^T$. Since we will use the expression for $r(z)$ in order to build LDDRK schemes, we prefer to write it as

$$r(z) = 1 + \gamma_1 z + \cdots + \gamma_s z^s, \tag{6}$$

where the explicit form of the coefficients γ_i for methods having up to six stages is

$$\begin{aligned} \gamma_1 &= \sum b_i, & \gamma_4 &= \sum b_i a_{ij} a_{jk} c_k \\ \gamma_2 &= \sum b_i c_i, & \gamma_5 &= \sum b_i a_{ij} a_{jk} a_{kl} c_l \\ \gamma_3 &= \sum b_i a_{ij} c_j, & \gamma_6 &= \sum b_i a_{ij} a_{jk} a_{kl} a_{lm} c_m. \end{aligned} \tag{7}$$

Note that some of the sums in (7) also appear in the order conditions. The method will be stable for all values of z such that $|r(z)| \leq 1$. If $s = p$, which is possible [5] only for $p \leq 4$, all coefficients γ_i are determined by the order conditions. That is why all classical RK methods have the same stability region.

Since the exact amplification factor is $r_e(z) = e^z$, expressing the ratio

$$\frac{r(z)}{r_e(z)} = \rho e^{-i\delta} \tag{8}$$

gives the dissipation error $1 - \rho$ and the phase (dispersion) error δ. One can then optimize the dissipation and dispersion errors, since they become functions of only the RK coefficients and z. To this end, Hu [2], for example, constricted the coefficients γ_i such that the integral $\int_0^Z |r(z) - r_e(z)|^2 \, dz$ be a minimum (with Z the limit of the optimization range), while still maintaining a certain order of accuracy. This leads to optimal values for the coefficients γ_i that are not determined by the order conditions. The schemes considered in [2] for which we search the $2N$-storage format are as follows:

(1) Second-order, five stage scheme (LDD25) with $\gamma_3 = 0.166558$, $\gamma_4 = 0.0395041$ and $\gamma_5 = 0.00781071$.

(2) Fourth-order, six stage scheme (LDD46) with $\gamma_5 = 0.0078105$, $\gamma_6 = 0.00132141$.

(3) Two-step fourth-order method (LDD56) for which the first step is a five-stage scheme with $\gamma_5 = 0.0036105$, and the second step is a six-stage scheme with $\gamma_5 = 0.0121101$ and $\gamma_6 = 0.00285919$.

3. FIVE-STAGE SCHEMES

In this case the relationships between the usual and the $2N$-storage RK coefficients are found to be

$$\begin{aligned}
a_{21} &= \beta_1, & a_{53} &= \alpha_4 a_{54} + \beta_3 \\
a_{32} &= \beta_2, & a_{52} &= \alpha_3 a_{53} + \beta_2 \\
a_{31} &= \alpha_2 a_{32} + \beta_1, & a_{51} &= \alpha_2 a_{52} + \beta_1 \\
a_{43} &= \beta_3, & b_5 &= \beta_5 \\
a_{42} &= \alpha_3 a_{43} + \beta_2, & b_4 &= \alpha_5 b_5 + \beta_4 \\
a_{41} &= \alpha_2 a_{42} + \beta_1, & b_3 &= \alpha_4 b_4 + \beta_3 \\
a_{54} &= \beta_4, & b_2 &= \alpha_3 b_3 + \beta_2 \\
& & b_1 &= \alpha_2 b_2 + \beta_1.
\end{aligned} \tag{9}$$

To obtain the second-order five-stage LDDRK method, the above relations are used to express the two order conditions that must be obeyed and the three additional constraints obtained by specifying $\gamma_3, \gamma_4, \gamma_5$ in terms of $\alpha_2, \ldots, \alpha_5$ and $\beta_1, \ldots, \beta_5$. This leads to a nonlinear system of five equations with nine unknowns, hence a four-parameter family of solutions will probably exist. To choose a solution one may, for example, impose the values for several variables and/or use additional equations. A solution thus obtained is presented below.

i	α	β	c
1	0.0	0.1	0.0
2	−0.6913065	0.75	0.1
3	−2.655155	0.7	0.3315201
4	−0.8147688	0.479313	0.4577796
5	−0.6686587	0.310392	0.8666528

4. SIX-STAGE SCHEMES

For six-stage schemes, the coefficients $a_{21}, \ldots, a_{54}, b_1, \ldots, b_4$ are still given by the relations in Eq. (9). The remaining coefficients are

$$\begin{aligned}
a_{65} &= \beta_5, & a_{62} &= \alpha_3 a_{63} + \beta_2 \\
a_{64} &= \alpha_5 a_{65} + \beta_4, & a_{61} &= \alpha_2 a_{62} + \beta_1 \\
a_{63} &= \alpha_4 a_{64} + \beta_3, & b_6 &= \beta_6 \\
& & b_5 &= \alpha_6 b_6 + \beta_5.
\end{aligned} \tag{10}$$

There are now eleven free coefficients $\alpha_2, \ldots, \alpha_6, \beta_1, \ldots, \beta_6$. To obtain the fourth order six stages LDDRK scheme the coefficients must obey the eight order conditions Eq. (3) and

the additional optimization constraints resulting from specification of γ_5, γ_6. The resulting nonlinear system has been solved upon imposing the value of one of the coefficients. One such solution is listed below.

i	α	β	c
1	0.0	0.1453095	0.0
2	−0.4919575	0.4653797	0.1453095
3	−0.8946264	0.4675397	0.3817422
4	−1.5526678	0.7795279	0.6367813
5	−3.4077973	0.3574327	0.7560744
6	−1.0742640	0.15	0.9271047

5. TWO-STEP SCHEMES

The two-step LDD56 scheme devised in [2] can be put in $2N$-storage format. The scheme has fourth order accuracy in both steps, and five/six stages in the first/second step. For the first step, the five stages imply nine free coefficients which are completely determined by the eight order conditions and the additional constraint $\gamma_5 = 0.0036105$. The second step is completely similar to LDD46, except for the values of the constants γ_5 and γ_6. We give here one set of coefficients for the first and second step, respectively.

i	α	β	c
1	0.0	0.2687454	0.0
2	−0.6051226	0.8014706	0.2687454
3	−2.0437564	0.5051570	0.5852280
4	−0.7406999	0.5623568	0.6827066
5	−4.4231765	0.0590065	1.1646854

i	α	β	c
1	0.0	0.1158488	0.0
2	−0.4412737	0.3728769	0.1158485
3	−1.0739820	0.7379536	0.3241850
4	−1.7063570	0.5798110	0.6193208
5	−2.7979293	1.0312849	0.8034472
6	−4.0913537	0.15	0.9184166

6. NUMERICAL RESULTS

In order to check the accuracy of the proposed methods, we use a system of nonlinear and non-autonomous first order differential equations

$$U' = \frac{1}{U} - \frac{Ve^{t^2}}{t^2} - t; \qquad V' = \frac{1}{V} - e^{t^2} - 2te^{-t^2} \tag{11}$$

together with the initial conditions $U(1) = 1$, $V(1) = e^{-1}$. The exact solution of this system is $U(t) = 1/t$, $V(t) = e^{-t^2}$. The system is solved numerically in double precision over the

TABLE 1
Error Norms and Their Ratios for Various Step Sizes for the Nonlinear System (11)

h	LDD46	R	LDD56	R	LDD25	R
1e-2	5.16e-8	17.8	4.31e-8	15.7	6.29e-7	5.9
5e-3	2.89e-9	16.9	2.74e-9	15.9	1.05e-7	5.2
2.5e-3	1.7e-10	16.5	1.73e-10	16.0	2.01e-8	4.7
1.25e-3	1.04e-11		1.08e-11		4.29e-9	

range $t \in [1, 1.4]$ using several step sizes h. In the limit $h \to \infty$ a decrease of h by a factor of two should decrease the error by a factor $R = 16$ for a fourth order method, and $R = 4$ for a second order method. The global error norms (computed as $|U - u| + |V - v|$) at $t = 1.4$ and their ratios, listed in Table 1, clearly show that LDD46 and LDD56 are fourth order accurate for nonlinear systems, while LDD25 is second order accurate.

Next, we use the schemes developed above to solve the convective wave equation, for which they have been optimized,

$$\frac{\partial U}{\partial t} + \frac{\partial U}{\partial x} = 0 \tag{12}$$

with initial conditions $U(t = 0) = 0.5e^{-x^2/9}$. The domain extends from $x = -50$ to $x = 450$, and the spatial discretization is obtained using eighth order central differences, with $\Delta x = 1$. In a first case the time step for all schemes has been chosen close to the stability limit of the fourth order six stage scheme (for stability and accuracy limits see [2]). For the second case, the time step is larger than the stability limit of LDD46 and close to the stability limit of LDD56. The maximum norm of the error $L_\infty = \max |u - U|$ at time $t = 400$ for the $2N$-storage schemes devised above is given in Table 2. Also given is the error for the fourth-order $2N$-storage scheme developed by Carpenter (CAR) [4] and the classical fourth-order four-stages RK (RK4) method which needs at least $3N$ storage. It turns out that for $h < 1.54$ the error for LDD56 is governed by the spatial discretization, no further decrease of the error being possible upon decreasing h. Figure 1 presents graphically the results for the first case (RK4 not shown), with the exact solution sampled at the same data points.

Different ways can be used to compare the relative efficiency of the methods. Among them, RK4 can be considered the most efficient if accuracy is not a concern, since it needs the smallest number of function evaluations to reach $t = 400$. When one compares the work needed to obtain a certain accuracy, however, the comparison favors the optimized methods.

TABLE 2
L_∞ Error Norms for the Advection Equation

Method	$h = 1.263$	$h = 1.543$
RK4	1.05e-1	1.41e-1
CAR	8.12e-2	1.01e-1
LDD25	3.77e-2	5.08e-2
LDD46	2.80e-2	–
LDD56	2.43e-2	2.44e-2

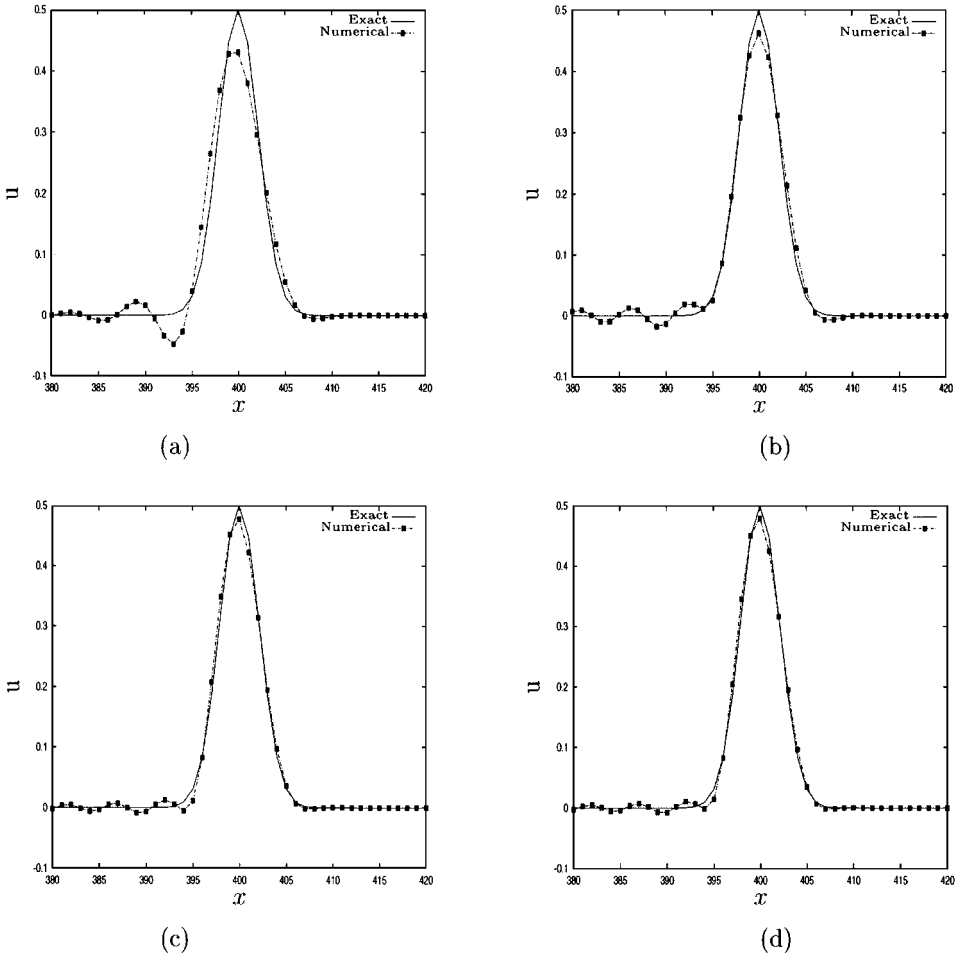

FIG. 1. Results obtained with $2N$-storage Runge-Kutta schemes for the linear advection equation. (a) Carpenter's 5-stage scheme, (b) LDD 2nd order 5 stage scheme, (c) LDD 4th order 6 stage scheme, (d) LDD two-step scheme.

For an error norm $L_\infty = 2.8\text{e-}2$, for example, where one is limited by the stability of LDD46, LDD25 needs a total of 2070 function evaluations (414 steps), LDD46 1914, CAR 3530 and RK4 3600, while the error for LDD56 at its stability limit where 1430 stages are needed is lower than the asked-for value. Considering the work required by RK4 as a reference, it follows that LDD25 is 1.74 times, LDD46 1.88 times, and LDD56 at least 2.52 times more efficient for this problem. The situation is slightly different when using the L_2 norm $\sqrt{1/N \sum_i (u_i - U_i)^2}$, this time LDD25 becoming more efficient than LDD46. Again for a value at the stability limit of RK 46, $L_2 = 3.4\text{e-}3$, one needs 1331 stages with LDD56, 1675 stages with LDD25, 1896 stages with LDD46, 2640 stages with RK4, and 2680 stages with CAR. The advantage of using optimized methods for wave-dominated problems is obvious.

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