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FOURTH-ORDER 2N-STORAGE RUNGE-KUTTA SCHEMES

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Abstract

A family of five-stage fourth-order Runge-Kutta schemes is derived; these schemes require only two storage locations. A particular scheme is identified that has desirable efficiency characteristics for hyperbolic and parabolic initial (boundary) value problems. This scheme is competitive with the classical fourth-order method (high-storage) and is considerably more efficient and accurate than existing third-order low-storage schemes.

Section 1: Introduction

Many problems of mathematical physics result in the numerical approximation of systems of coupled ordinary differential equations (ODE's). The technique for integrating the equations depends on, among other things, the desired accuracy, efficiency, robustness, and simplicity. For the ODE's that result from the direct simulation of the equations of fluid dynamics, the overriding consideration is often the availability of fast memory. A numerical integration technique that minimizes memory storage is essential and can be formulated with a Runge-Kutta (RK) methodology.

Williamson [1] showed that all second-order and some third-order RK schemes can be cast in a 2N-storage format, where N is the dimension of the system of ODE's. He also showed that (except for certain exceptional cases that involve specific forms of the function to be integrated) the four-stage fourth-order RK schemes cannot be put into 2N-storage format. Fyfe [2] showed that all four-stage fourth-order RK schemes can be implemented in 3N-storage locations. In spite of the reduced accuracy, for many applications the methods of choice are the 2N-storage third-order RK schemes.

Although the principal motivation of this work is to derive schemes of 2N storage, both the accuracy and efficiency also determine the practical utility of any scheme. For example, a fourth-order 2N-storage scheme with a vanishingly small stability envelope is of little practical value. The

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efficiency of an RK scheme is determined by the absolute size of the stability domain relative to the number of stages needed to implement the scheme. Typically, RK schemes that utilize the minimum number of stages necessary to achieve a given order of accuracy are used because they minimize the absolute workload for a given order of accuracy. Verner [3], however, demonstrated that the 13-stage eighth-order scheme is more efficient than the 12-stage eighth-order scheme. Similarly, Sharp et al. [4] showed that the efficiency of many existing fifth-, sixth-, and seventh-order RK schemes can be increased by including additional stages while retaining the same order of accuracy. The additional stages are used to optimize the absolute stability domain and increase the relative efficiency of each stage.

A five-stage fourth-order RK scheme that satisfies the 2N-storage constraint is sought. The scheme should have the largest absolute linear stability envelope and the lowest truncation error possible. In section 2, we describe the conventional and the 2N-storage RK nomenclature. In section 3, we derive the complete set of three-stage third-order (3,3) RK schemes that can be cast in 2N-storage format. We then introduce a new set of four-stage third-order (4,3) RK schemes that are 2N-storage schemes. In section 4, we derive the new five-stage fourth-order (5,4) RK schemes that require 2N storage. In section 5, we compare all schemes for efficiency, accuracy, and simplicity and then draw conclusions in regard to the utility of the new schemes.

Section 2: Runge-Kutta Nomenclature

We are concerned with the numerical solution of the initial value problem

$$\frac{dU}{dt} = F[t, U(t)]; \quad U(t_0) = U_0$$

Assume that the discrete approximation is made with an M-stage explicit RK scheme. The implementation over a time step h is accomplished by

$$\begin{aligned} k_1 &= F(t_0, U^0) \\ k_i &= F\left(t_0 + c_i h,\ U^0 + h\sum_{j=1}^{i-1} a_{i,j} k_j\right) \qquad i = 2, ..., M \\ U^1 &= U^0 + h\sum_{j=1}^{M} b_j k_j \end{aligned}$$

where $U^0 = U(t_0)$ and $U^1 = U(t_0 + h)$ and the fixed scalars $a_{i,j}, b_j, c_i$ are the coefficients of the RK formula.

Butcher [5] developed a succinct nomenclature for writing all RK schemes in terms of the fixed scalar coefficients $a_{i,j}, b_j, c_i$. The general, M-stage, explicit RK scheme can be expressed as

$$
\begin{array}{c|cccc}
c_1 & & & & \\
\cdot & a_{2,1} & & & \\
\cdot & \cdot & \cdot & & \\
\cdot & \cdot & \cdot & \cdot & \\
c_M & a_{M,1} & \cdot & \cdot & a_{M,M-1} \\
\hline
 & b_1 & \cdot & \cdot & \cdot \quad b_M
\end{array}
$$

The entries in the first column (c_i, $i = 1, M$) are the intermediate time levels. The coefficients $a_{i,j}$ are the intermediate weights of each RK stage i. By definition, $c_i = \sum_{j=1}^{M} a_{i,j}$ and $c_1 = 0$ for the explicit self-starting case. The last row (b_j, $j = 1, M$) are the weights of the final stage.

To devise low-storage RK schemes, Williamson and Fyfe exploit the technique of leaving useful information in the storage register. Each successive stage is written onto the same register without zeroing the previous value. Thus, the M-stage algorithm becomes

$$
\begin{array}{rcrcl}
dU_j & = & A_j dU_{j-1} & + & hF(U_j) \\
U_j & = & U_{j-1} & + & B_j dU_j \qquad j = 1, M
\end{array}
$$

So that the algorithm is self-starting, $A_1 = 0$. Only the dU and U vectors must be stored, which results in a 2N-storage algorithm.

Williamson [1] first presented the relationship between the general RK scheme and the 2N-storage scheme. Specifically, the following equations provide the relationship between the 2N-storage variables A_j and B_j and the conventional RK variables $a_{i,j}, b_j$, and c_i:

$$
\begin{array}{rcll}
B_j & = & a_{j+1,j} & (j \neq M) \\
B_M & = & b_M & \\
A_j & = & (b_{j-1} - B_{j-1})/b_j & (j \neq 1, b_j \neq 0) \\
A_j & = & (a_{j+1,j-1} - c_j)/B_j & (j \neq 1, b_j = 0)
\end{array}
\qquad (1)
$$

The precise values of A_j and B_j that are required to yield a higher order scheme remain to be determined. Third-order RK schemes are the lowest order schemes for which the determination of 2N-storage is nontrivial. We begin by demonstrating the procedure for finding high-order 2N storage RK schemes for the third-order case.

Section 3: Third-Order Runge-Kutta Methods

For a third-order Runge-Kutta scheme, at least three stages are required. The general Butcher array diagram for the three-stage explicit scheme is written as

$$
\begin{array}{c|ccc}
c_1 & & & \\
c_2 & a_{2,1} & & \\
c_3 & a_{3,1} & a_{3,2} & \\
\hline
 & b_1 & b_2 & b_3
\end{array}
$$

For third-order accuracy, seven constraints between the coefficients $a_{i,j}$, b_j, and c_i must be satisfied [5]:

$$\sum_{i=1}^{3} b_i = 1^{(1)} \quad ; \quad \sum_{i=1}^{3} b_i c_i = \frac{1}{2}^{(2)} \quad ; \quad \sum_{i=1}^{3} b_i c_i^2 = \frac{1}{3}^{(3)} \quad ; \quad \sum_{i,j=1}^{3} b_i a_{i,j} c_j = \frac{1}{6}^{(3)} \tag{2}$$

and

$$c_i = \sum_{j=1}^{3} a_{i,j} \qquad i = 1,3 \tag{3}$$

The superscripts on each of equations (2) indicate the order of accuracy that the constraint equation governs. If equations (2) and (3) are solved for the seven nonlinear algebraic equations in nine unknowns, then three solutions result, the most general of which involves a two-parameter family. If c_2 and c_3 are defined as the free parameters ($c_1 = 0$ for explicit RK schemes), then the following is true for case 1 (for which $c_2 \neq 0, 2/3$, or c_3 when $c_3 \neq 0$):

$$b_2 = \frac{c_3 - \frac{2}{3}}{2c_2(c_3 - c_2)} \quad ; \quad b_3 = \frac{\frac{2}{3} - c_2}{2c_3(c_3 - c_2)} \quad ; \quad b_1 = 1 - b_2 - b_3 \quad ; \quad a_{3,2} = \frac{1}{6b_3c_2} \tag{4}$$

Two additional solutions account for the solution points excluded from case 1. Exceptional solutions exist when $c_2 = 2/3$ or $c_2 = c_3$ ($c_2 = 0$ is an uninteresting case). These solutions are governed by

$$b_2 = \frac{3}{4} \quad ; \quad b_1 = \frac{1}{4} - b_3 \quad ; \quad a_{3,2} = \frac{1}{4b_3} \tag{5}$$

for case 2 (for which $c_2 = \frac{2}{3}$, $c_3 = 0$ and b_3 is an arbitrary nonzero number), and

$$b_2 = \frac{1}{4} \quad ; \quad b_1 = \frac{3}{4} - b_3 \quad ; \quad a_{3,2} = \frac{1}{4b_3} \tag{6}$$

for case 3 (for which $c_2 = c_3 = \frac{2}{3}$ and b_3 is an arbitrary non-zero number). Equations (4) through (6) span the complete set of (3,3) RK schemes.

The linear stability envelope for the (3,3) RK schemes is determined by

$$\mathbf{G} = 1 + \left(\sum_{i=1}^{3} b_i\right)\mathbf{Z} + \left(\sum_{i=1}^{3} b_i c_i\right)\mathbf{Z}^2 + \left(\sum_{i,j=1}^{3} b_i a_{ij} c_j\right)\mathbf{Z}^3 \;=\; 1 + \mathbf{Z} + \frac{1}{2}\mathbf{Z}^2 + \frac{1}{6}\mathbf{Z}^3$$

where $\mathbf{Z}$ is a complex number that is considered in detail later and $\mathbf{G}$ is the amplification matrix. The coefficients of $\mathbf{G}$ are precisely the linear constraint equations defined in equation (2); thus, all (3,3) RK schemes have identical linear stability envelopes. The nonlinear accuracy, however, will depend on the specific choice of scheme and will be problem dependent. Numerous different methods for choosing a scheme based on accuracy criteria are summarized elsewhere [6].

Not all solutions defined in equations (4) through (6) can be put into the 2N-storage format. The 2N-storage condition imposes independent constraints in addition to those in equations (2) and (3).

To demonstrate this, we establish the Butcher array form of the 2N-storage scheme. The original Butcher array is expanded in terms of the 2N-storage variables A_j and B_j to obtain

$$\begin{array}{c|ccc} 0 & & & \\ c_2 & a_{2,1} & & \\ c_3 & a_{3,1} & a_{3,2} & \\ \hline & b_1 & b_2 & b_3 \end{array} \quad = \quad \begin{array}{c|ccc} 0 & & & \\ B_1 & B_1 & & \\ B_1 + B_2(A_2+1) & [A_2 B_2 + B_1] & B_2 & \\ \hline & [A_2(A_3 B_3 + B_2) + B_1] & [A_3 B_3 + B_2] & B_3 \end{array}$$

From the relationships defined in equations (1), the values $a_{2,1}$, $a_{3,2}$, b_3, b_2, and b_1 are immediately determined by the values of B_1, B_2, B_3, A_3, and A_2, respectively. By definition, the conditions $c_i = \sum_{j=1}^{3} a_{i,j}$ will automatically be satisfied. The only condition that is not immediately satisfied involves $a_{3,1}$, or specifically $a_{31} = [A_2 B_2 + B_1]$. By adjusting the free parameters in each of the three general solutions, this final constraint can be satisfied. For case 1, for which $c_2 \neq 0, 2/3$, or c_3 and $c_3 \neq 0$, a one-parameter family of solutions results. If we define

$$\begin{aligned} z_1 &= \sqrt{(36c_2^4 + 36c_2^3 - 135c_2^2 + 84c_2 - 12)} \\ z_2 &= 2c_2^2 + c_2 - 2 \\ z_3 &= 12c_2^4 - 18c_2^3 + 18c_2^2 - 11c_2 + 2 \\ z_4 &= 36c_2^4 - 36c_2^3 + 13c_2^2 - 8c_2 + 4 \\ z_5 &= 69c_2^3 - 62c_2^2 + 28c_2 - 8 \\ z_6 &= 34c_2^4 - 46c_2^3 + 34c_2^2 - 13c_2 + 2 \end{aligned} \tag{7}$$

then the one-parameter family is given by

$$\begin{aligned} B_1 &= c_2 \\ B_2 &= \frac{12c_2(c_2-1)(3z_2-z_1) - (3z_2-z_1)^2}{144c_2(3c_2-2)(c_2-1)^2} \\ B_3 &= \frac{-24(3c_2-2)(c_2-1)^2}{(3z_2-z_1)^2 - 12c_2(c_2-1)(3z_2-z_1)} \\ A_2 &= \frac{-(6c_2^2-4c_2+1)z_1 + 3z_3}{(2c_2+1)z_1 - 3(c_2+2)(2c_2-1)^2} \\ A_3 &= \frac{-z_4 z_1 + 108(2c_2-1)c_2^5 - 3(2c_2-1)z_5}{24z_1c_2(c_2-1)^4 + 72c_2z_6 + 72c_2^6(2c_2-13)} \end{aligned} \tag{8}$$

provided that none of the respective denominators vanishes. A scheme that both eliminates the square roots and is close to the optimum truncation error was identified by Williamson [1] as

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{3} & \frac{1}{3} & & \\ \frac{3}{4} & -\frac{3}{16} & \frac{15}{16} & \\ \hline & \frac{1}{6} & \frac{3}{10} & \frac{8}{15} \end{array} \Rightarrow \begin{array}{c|c} A_1 & B_1 \\ A_2 & B_2 \\ A_3 & B_3 \end{array} = \begin{array}{c|c} 0 & \frac{1}{3} \\ -\frac{5}{9} & \frac{15}{16} \\ -\frac{153}{128} & \frac{8}{15} \end{array} \qquad (9)$$

This scheme, which is widely used, will be referred to as the (3,3) 2N-storage scheme of Williamson in the remainder of this paper.

For case 2, for which $c_2 = \frac{2}{3}$, $c_3 = 0$, and b_3 is an arbitrary nonzero number, we find a 2N-storage solution for $b_3 = -\frac{1}{3}$ that results in the scheme

$$\begin{array}{c|ccc} 0 & & & \\ \frac{2}{3} & \frac{2}{3} & & \\ 0 & \frac{3}{4} & -\frac{3}{4} & \\ \hline & \frac{7}{12} & \frac{3}{4} & -\frac{1}{3} \end{array} \Rightarrow \begin{array}{c|c} 0 & \frac{2}{3} \\ -\frac{1}{9} & -\frac{3}{4} \\ -\frac{9}{2} & -\frac{1}{3} \end{array}$$

For case 3, for which $c_2 = c_3 = \frac{2}{3}$ and b_3 is an arbitrary nonzero number, we find a 2N-storage solution for $b_3 = \frac{1}{3}$ that results in the scheme

$$\begin{array}{c|ccc} 0 & & & \\ \frac{2}{3} & \frac{2}{3} & & \\ \frac{2}{3} & -\frac{1}{12} & \frac{3}{4} & \\ \hline & \frac{1}{4} & \frac{5}{12} & \frac{1}{3} \end{array} \Rightarrow \begin{array}{c|c} 0 & \frac{2}{3} \\ -1 & \frac{3}{4} \\ -1 & \frac{1}{3} \end{array}$$

Because the 2N-storage schemes are a subset of the general (3,3) RK scheme solutions, they too have identical linear stability envelopes.

To obtain different linear stability characteristics for third-order RK schemes, additional stages must be used. One additional stage adds one constraint equation ($c_4 = \sum_{j=1}^{4} a_{4,j}$) to the seven nonlinear equations and adds five new variables. The general solution which involves eight equations in fourteen variables, is a six parameter family. If 2N-storage is required, then three additional equations must be satisfied, which eliminates three of the six free parameters. The general four-stage third-order (4,3) RK solution that involves 2N-storage can be expressed as a three-parameter family. A two-parameter family may be generated by enforcing the linear, fourth-order constraint. None of these general expressions are presented here because of their complexity.

If third-order accuracy is achieved in four stages instead of three, then the required work per time step is increased by one third. By enforcing the linear, fourth-order constraint, the increased stability envelope of the (4,3) RK schemes more than offsets this additional work. The (4,3) schemes are more efficient per unit time, which is consistent with the work of Sharp et al. [4]. An extensive study of the stability domains of the (4,3) RK schemes shows that a nearly optimal scheme can be obtained by setting

$$\begin{aligned} G &= 1+\left(\sum_{i=1}^{4} b_i\right) Z + \left(\sum_{i=1}^{4} b_i c_i\right) Z^2 + \left(\sum_{i,j=1}^{4} b_i a_{ij} c_j\right) Z^3 + \left(\sum_{i,j,k=1}^{4} b_i a_{ij} a_{jk} c_k\right) Z^4 \\ &= 1 + Z + \frac{1}{2}Z^2 + \frac{1}{6}Z^3 + \frac{1}{24}Z^4 \end{aligned}$$

Note that these schemes are third-order accurate for the nonlinear problem but fourth-order accurate for the linear problem. Three third-order schemes that satisfy the 2N-storage constraint in four stages and have a nearly optimal stability envelope are now presented. If we set $c_2 = c_3$, then

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{3} & \frac{1}{3} & & & \\ \frac{1}{3} & -\frac{5}{12} & \frac{3}{4} & & \\ 1 & \frac{1}{4} & \frac{1}{12} & \frac{2}{3} & \\ \hline & 0 & \frac{1}{3} & \frac{5}{12} & \frac{1}{4} \end{array} \Rightarrow \begin{array}{r|c} 0 & \frac{1}{3} \\ -1 & \frac{3}{4} \\ -1 & \frac{2}{3} \\ -1 & \frac{1}{4} \end{array} \qquad (10)$$

If we set $c_3 = c_4$, then

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{1}{4} & \frac{1}{4} & & & \\ \frac{11}{12} & -\frac{11}{36} & \frac{11}{9} & & \\ \frac{11}{12} & \frac{419}{396} & -\frac{16}{9} & \frac{18}{11} & \\ \hline & -\frac{1}{11} & \frac{3}{4} & \frac{17}{66} & \frac{1}{12} \end{array} \Rightarrow \begin{array}{r|c} 0 & \frac{1}{4} \\ -\frac{5}{11} & \frac{11}{9} \\ -\frac{11}{6} & \frac{18}{11} \\ -\frac{182}{11} & \frac{1}{12} \end{array} \quad \text{or} \quad \begin{array}{c|cccc} 0 & & & & \\ \frac{19}{36} & \frac{19}{36} & & & \\ \frac{3}{4} & -\frac{51}{76} & \frac{27}{19} & & \\ \frac{3}{4} & \frac{19}{36} & 0 & \frac{2}{9} & \\ \hline & \frac{13}{57} & \frac{27}{76} & \frac{1}{6} & \frac{1}{4} \end{array} \Rightarrow \begin{array}{r|c} 0 & \frac{19}{36} \\ -\frac{205}{243} & \frac{27}{19} \\ -\frac{243}{38} & \frac{2}{9} \\ -\frac{2}{9} & \frac{1}{4} \end{array}$$

If we demand that the intermediate time levels c_j be monitonically increasing, then

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{9} & \frac{1}{9} & & & \\
\frac{4}{9} & -\frac{11}{36} & \frac{3}{4} & & \\
\frac{6}{9} & -\frac{1}{12} & \frac{7}{20} & \frac{2}{5} & \\
\hline
 & -1 & 2 & -\frac{5}{4} & \frac{5}{4}
\end{array}
\Rightarrow
\begin{array}{c|c}
0 & \frac{1}{9} \\
-\frac{5}{9} & \frac{3}{4} \\
-1 & \frac{2}{5} \\
-\frac{33}{25} & \frac{5}{4}
\end{array}
\quad \text{or} \quad
\begin{array}{c|cccc}
0 & & & & \\
\frac{3}{9} & \frac{3}{9} & & & \\
\frac{5}{9} & -\frac{5}{18} & \frac{5}{6} & & \\
\frac{8}{9} & \frac{41}{90} & -\frac{1}{6} & \frac{3}{5} & \\
\hline
 & \frac{3}{20} & \frac{1}{4} & \frac{7}{20} & \frac{1}{4}
\end{array}
\Rightarrow
\begin{array}{c|c}
0 & \frac{1}{3} \\
-\frac{11}{15} & \frac{5}{6} \\
-\frac{5}{3} & \frac{3}{5} \\
-1 & \frac{1}{4}
\end{array}
$$

For problems in which third-order temporal accuracy is sufficient, these new schemes should be considered because of their larger stability envelope.

Section 4: Fourth-Order Runge-Kutta

Twelve nonlinear algebraic equations in fourteen variables determine the solution to the four-stage fourth-order (4,4) RK schemes. Five general solutions exist: one that involves two free parameters and four that involve one free parameter, covering the special roots excluded by the first. (See Butcher for the general solutions [5].) Fyfe [2] demonstrated that all cases can be implemented in the 3N-storage format. Williamson [1] demonstrated that they could not, in general, be implemented in the 2N-storage format. The 2N-storage constraint adds three additional equations that cannot be satisfied by any of the five general solutions.

By increasing the number of stages, additional degrees of freedom are generated that can be used to satisfy all fourth-order and 2N-storage constraint equations. The five-stage fourth-order (5,4) RK scheme may be expressed in Butcher and 2N-storage form as

$$
\begin{array}{c|ccccc}
c_1 & & & & & \\
c_2 & a_{2,1} & & & & \\
c_3 & a_{3,1} & a_{3,2} & & & \\
c_4 & a_{4,1} & a_{4,2} & a_{4,3} & & \\
c_5 & a_{5,1} & a_{5,2} & a_{5,3} & a_{5,4} & \\
\hline
 & b_1 & b_2 & b_3 & b_4 & b_5
\end{array}
\Rightarrow
\begin{array}{c|c}
A_1 & B_1 \\
A_2 & B_2 \\
A_3 & B_3 \\
A_4 & B_4 \\
A_5 & B_5
\end{array}
$$

For explicit self-starting schemes, $c_1 = 0$, and $A_1 = 0$. For any (5,4) RK scheme, the nonlinear accuracy constraints are

$$
\begin{array}{c}
\sum_{i=1}^{5} b_i = 1^{(1)} \;;\; \sum_{i=1}^{5} b_i c_i = \frac{1}{2}^{(2)} \;;\; \sum_{i=1}^{5} b_i c_i^2 = \frac{1}{3}^{(3)} \;;\; \sum_{i,j=1}^{5} b_i a_{i,j} c_j = \frac{1}{6}^{(3)} \\
\sum_{i=1}^{5} b_i c_i^3 = \frac{1}{4}^{(4)} \;;\; \sum_{i,j=1}^{5} b_i c_i a_{i,j} c_j = \frac{1}{8}^{(4)} \;;\; \sum_{i,j=1}^{5} b_i a_{i,j} c_j^2 = \frac{1}{12}^{(4)} \;;\; \sum_{i,j,k=1}^{5} b_i a_{i,j} a_{j,k} c_k = \frac{1}{24}^{(4)}
\end{array}
\quad (11)
$$

and

$$c_i = \sum_{j=1}^{5} a_{i,j} \quad i = 1,5$$

Again, the superscripts on equations (11) indicate the order of accuracy from which the constraint was obtained. Note that the first four are similar to those needed in the (3,3) and (4,3) RK schemes; the last four are specific to the fourth-order accuracy condition. These 13 constraint equations involve 20 unknowns (five b_i's, five c_i's, and ten $a_{i,j}$'s), which represents at least a seven-parameter family of schemes.

The relationships between the original RK variables $a_{i,j}, b_j, c_i$ and the 2N-storage variables A_j, B_j are

$$\begin{aligned}
a_{2,1} &= B_1, & c_1 &= 0 \\
a_{3,1} &= A_2B_2 + B_1, & c_2 &= B_1 \\
a_{3,2} &= B_2, & c_3 &= B_1 + B_2(A_2+1) \\
a_{4,1} &= A_2(A_3B_3 + B_2) + B_1, & c_4 &= B_1 + B_2(A_2+1) + B_3[A_3(A_2+1)+1] \\
a_{4,2} &= A_3B_3 + B_2, & c_5 &= B_1 + B_2(A_2+1) + B_3[A_3(A_2+1)+1] + B_4\{A_4[A_3(A_2+1)+1]+1\} \\
a_{4,3} &= B_3, & b_1 &= A_2\{A_3[A_4(A_5B_5 + B_4) + B_3] + B_2\} + B_1 \\
a_{5,1} &= A_2[A_3(A_4B_4 + B_3) + B_2] + B_1, & b_2 &= A_3[A_4(A_5B_5 + B_4) + B_3] + B_2 \\
a_{5,2} &= A_3(A_4B_4 + B_3) + B_2, & b_3 &= A_4(A_5B_5 + B_4) + B_3 \\
a_{5,3} &= A_4B_4 + B_3, & b_4 &= A_5B_5 + B_4 \\
a_{5,4} &= B_4, & b_5 &= B_5
\end{aligned}$$

If the (5,4) RK scheme is constrained to a 2N-storage format, six additional constraint equations are produced. Specifically, from the relationships defined in equations (1), the values $a_{2,1}$, $a_{3,2}$, $a_{4,3}$, $a_{5,4}$, b_5, b_4, b_3, b_2, and b_1 are immediately determined by the values of B_1, B_2, B_3, B_4, B_5, A_5, A_4, A_3, and A_2, respectively. ($A_1 = 0$.) Again, by definition, the conditions $c_i = \sum_{j=1}^{5} a_{i,j}$ are automatically satisfied. The constraint equations that are not immediately satisfied are those that involve the values $a_{3,1}$, $a_{4,1}$, $a_{4,2}$, $a_{5,1}$, $a_{5,2}$, and $a_{5,3}$. These six additional equations yield a system of 19 constraint equations in 20 unknowns. Assuming a solution exists, in general, there is a one parameter family of solutions. The general answer is not forthcoming due to the complexity of the equations.

We can determine specific solutions to the 19 equations in 20 unknowns. Frequently, we can simplify the equations considerably by assuming special forms of the coefficients c_i or A_i. The algebra simplifies considerably if we assume that $c_2 = c_3$. This assumption eliminates the one degree of freedom in the general solution but produces an exact analytic solution. The Butcher diagram for this case becomes

$$
\begin{array}{c|ccccc}
\frac{2}{3}+\frac{\sqrt[3]{2}}{3}+\frac{2^{2/3}}{6} & \frac{2}{3}+\frac{\sqrt[3]{2}}{3}+\frac{2^{2/3}}{6} & & & & \\
\frac{2}{3}+\frac{\sqrt[3]{2}}{3}+\frac{2^{2/3}}{6} & \frac{\sqrt[3]{2}}{3}+\frac{2^{2/3}}{3}+\frac{1}{2} & -\frac{2^{2/3}}{6}+\frac{1}{6} & & & \\
\frac{1}{3}-\frac{\sqrt[3]{2}}{3}-\frac{2^{2/3}}{6} & -\frac{2^{2/3}}{6}+\frac{1}{6} & \frac{\sqrt[3]{2}}{3}+\frac{2^{2/3}}{3}+\frac{1}{2} & -\frac{1}{3}-\frac{2\sqrt[3]{2}}{3}-\frac{2^{2/3}}{3} & & \\
1 & \frac{\sqrt[3]{2}}{3}+\frac{2^{2/3}}{3}+\frac{1}{2} & -\frac{2^{2/3}}{6}+\frac{1}{6} & & \frac{1}{3}-\frac{\sqrt[3]{2}}{3}-\frac{2^{2/3}}{6} & \\
\hline
 & \frac{1}{3}+\frac{\sqrt[3]{2}}{6}+\frac{2^{2/3}}{12} & \frac{1}{3}+\frac{\sqrt[3]{2}}{6}+\frac{2^{2/3}}{12} & -\frac{2^{2/3}}{6}-\frac{\sqrt[3]{2}}{3}-\frac{1}{6} & \frac{1}{6}-\frac{\sqrt[3]{2}}{6}-\frac{2^{2/3}}{12} & \frac{1}{3}+\frac{\sqrt[3]{2}}{6}+\frac{2^{2/3}}{12}
\end{array}
$$

The 2N-storage array becomes

$$
\begin{array}{c|c}
A_1 & B_1 \\
A_2 & B_2 \\
A_3 & B_3 \\
A_4 & B_4 \\
A_5 & B_5
\end{array}
=
\begin{array}{c|c}
0 & 2/3+\frac{\sqrt[3]{2}}{3}+\frac{2^{2/3}}{6} \\
-1 & -\frac{2^{2/3}}{6}+1/6 \\
-1/3+\frac{2^{2/3}}{6}-\frac{2\sqrt[3]{2}}{3} & -1/3-\frac{2\sqrt[3]{2}}{3}-\frac{2^{2/3}}{3} \\
-\sqrt[3]{2}-2^{2/3}-2 & 1/3-\frac{\sqrt[3]{2}}{3}-\frac{2^{2/3}}{6} \\
-1+\sqrt[3]{2} & 1/3+\frac{\sqrt[3]{2}}{6}+\frac{2^{2/3}}{12}
\end{array}
$$

Because $\sum_{i,j,k,l=1}^{5} b_i a_{ij} a_{jk} a_{kl} c_l = -(\frac{1}{72}+\frac{\sqrt[3]{2}}{72}+\frac{2^{2/3}}{72})$, the linear stability envelope is found by considering

$$
\mathbf{G} = 1+\mathbf{Z}+\frac{1}{2}\mathbf{Z}^2+\frac{1}{6}\mathbf{Z}^3+\frac{1}{24}\mathbf{Z}^4-\left(\frac{1}{72}+\frac{\sqrt[3]{2}}{72}+\frac{2^{2/3}}{72}\right)\mathbf{Z}^5
$$

where $\sum_{i,j,k,l=1}^{5} b_i a_{ij} a_{jk} a_{kl} c_l \approx \frac{-1}{20}$. A second analytic solution has been obtained by setting all values of the $A_j = -1$ for $j = 2, 5$. The 2N-storage array for this case becomes

$$
\begin{array}{c|c}
A_1 & B_1 \\
A_2 & B_2 \\
A_3 & B_3 \\
A_4 & B_4 \\
A_5 & B_5
\end{array}
=
\begin{array}{c|c}
0 & \frac{64B_4{}^2-32B_4+1}{96B_4{}^2-60B_4} \\
-1 & -\frac{64B_4{}^3-80B_4{}^2+25B_4}{64B_4{}^2-32B_4+1} \\
-1 & \frac{-1}{16B_4{}^2-10B_4} \\
-1 & B_4 \\
-1 & \frac{4B_4-1}{12B_4}
\end{array}
$$

for which the amplification matrix is

$$
\mathbf{G} = 1+\mathbf{Z}+\frac{1}{2}\mathbf{Z}^2+\frac{1}{6}\mathbf{Z}^3+\frac{1}{24}\mathbf{Z}^4+\left(\frac{B_4-\frac{1}{4}}{72B_4}\right)\mathbf{Z}^5
$$

(The Butcher array is not presented here because of the small stability envelope of this scheme.) The coefficient B_4 is defined as $B_4 = \frac{5}{24} - \sqrt[3]{X} - \frac{1}{576\sqrt[3]{X}}$ with $X = \frac{163}{13824} + \frac{\sqrt{82}}{768}$. Because $\frac{B_4-\frac{1}{4}}{72B_4} \approx \frac{1}{20}$, the amplification matrix becomes $\mathbf{G} \approx 1+\mathbf{Z}+\frac{1}{2}\mathbf{Z}^2+\frac{1}{6}\mathbf{Z}^3+\frac{1}{24}\mathbf{Z}^4+\left(\frac{1}{20}\right)\mathbf{Z}^5$. Neither of the two analytic solutions has a desirable stability envelope, as we shall see later. The first is of marginal value, and the second is extremely small. However, they are of some value because they provide good initial guesses for determining numerical roots.

In general, we must resort to a numerical solution of the 19 equations in 20 unknowns. The ultimate goal is a scheme that has an optimal stability envelope. We can constrain the last degree of freedom in the general system by demanding that the resulting scheme be optimal, which produces a system with 20 equations and 20 unknowns.

To define the optimal constraint, we begin with the amplification matrix for the (5,4) RK scheme, which is given by

$$\mathbf{G} = 1 + \left(\sum_{i=1}^{5} b_i\right)\mathbf{Z} + \left(\sum_{i=1}^{5} b_i c_i\right)\mathbf{Z}^2 + \left(\sum_{i,j=1}^{5} b_i a_{ij} c_j\right)\mathbf{Z}^3 + \left(\sum_{i,j,k=1}^{5} b_i a_{ij} a_{jk} c_k\right)\mathbf{Z}^4 + \left(\sum_{i,j,k,l=1}^{5} b_i a_{ij} a_{jk} a_{kl} c_l\right)\mathbf{Z}^5$$

A particular scheme can be defined as being optimal when its stability envelope encompasses a useful portion of the complex plane that is as large as possible for a particular choice of the complex matrix $\mathbf{Z}$. This definition of optimality is problem dependent and depends on the structure of the eigenvalues of the system of ODE's being integrated.

We now focus specifically on hyperbolic and parabolic partial differential equations (PDE's), for which the (5,4) 2N-storage RK schemes will be advantageous. A model equation that produces an eigenstructure representative of the equations of fluid mechanics is $U_t + aU_x = \alpha U_{xx}$. If we choose spatial operators for the U_x and U_{xx} terms, this equation reduces to a system of ODE's. The complex matrix $\mathbf{Z}$ can now be interpreted to represent combinations of the inviscid and viscous stability characteristics. Figure 1 shows a parametric study of the stability envelope as a function of the CFL number $\left(\lambda = \frac{a\Delta t}{\Delta x}\right)$ and the viscous CFL number $\left(\lambda = \frac{\alpha\Delta t}{(\Delta x)^2}\right)$, as determined from the amplification matrix $\mathbf{G}$. Regions toward the origin represent stable regions for the scheme, and the upper right portion of the plot represents the unstable regions. The spatial operator used for both the inviscid and viscous operators was the sixth-order compact scheme [7]; however, similar conclusions could have been reached with a second-order or a Fourier method. (See the appendix for more details.) The parameter α is defined as $\alpha = \sum_{i,j,k,l=1}^{5} b_i a_{ij} a_{jk} a_{kl} c_l$. By adjusting $-1 \leq \alpha \leq 1$, large stability envelopes are obtained for values of $\alpha \approx 0$. Figure 2 shows a more refined plot of values $\frac{1}{280} \leq \alpha \leq \frac{1}{120}$. Note that all curves have a similar structure but that no one curve simultaneously maximizes the inviscid (imaginary axis) and viscous (real axis) stability limits. Further inspection reveals that the maximum inviscid stability occurs at $\alpha = \frac{1}{100\sqrt{2}}$; the viscous stability limit occurs at $\alpha \approx \frac{1}{244}$. The value $\alpha = \frac{1}{200}$ provides a compromise between the two extremes. Caution should be exercised in using values of α near $\frac{1}{100\sqrt{2}}$ because the inviscid stability limit in the case of very small viscous CFL values may change dramatically with small changes in α. Figure 3 shows the stability limits for the (3,3) RK scheme, the (4,4) RK scheme, and three (5,4) RK schemes that are functions of the parameter α. Figure 3 illustrates why the analytic schemes presented earlier do not have desirable stability characteristics. The stability envelope for the analytic case $\alpha \approx \frac{-1}{20}$ is about half the size of the optimal $\alpha = \frac{1}{200}$; the analytic case $\alpha \approx \frac{1}{20}$ has a vanishingly small inviscid stability limit.

The optimal value $\alpha = \frac{1}{200}$ is used to provide the 20th nonlinear equation in 20 unknowns. The general solution is no longer a one-parameter family and, because of the nonlinearity in the equations, is not unique. Specifically, the 20th equation becomes

$$\sum_{i,j,k,l=1}^{5} b_i a_{i,j} a_{j,k} a_{k,l} c_l = \frac{1}{200} \tag{13}$$

To solve the 20 equations in 20 unknowns, the partial linearity of the system is exploited to reduce it to nine equations in the variables $A_j, B_j, j = 1,5$ with $A_1 = 0$. This procedure is equivalent to substituting the values of $a_{i,j}$, b_j, and c_i found in equations (12) into equations (11) and (13). The Jacobian of the system is calculated analytically, and then a factored secant update is used to obtain a solution. Because the equations are nonlinear, multiple roots exist. Some roots were found with the analytic solutions as an initial guess. Others were found with random initial guesses.

At least nine real roots have been identified that satisfy all nine equations. In general, none of these nine formulations is optimal for every problem. We can, however, use heuristic arguments to identify certain roots as less desirable. Verner [3] cites several theoretical considerations that should be used in determining desirable roots. Those that are relevant to this work are

I Each intermediate time level ($c_i, i = 1,5$) should be in the interval [0,1] to control the effect of rapidly changing derivatives.

II The weights of the $b_j, j = 1,5$ should be positive.

III Coefficients should incorporate rational numbers requiring a small number of digits.

Four of the nine roots satisfy condition I; only one satisfies conditions I and II. We were not able to express any of the roots in terms of "convenient" rational numbers.

Table 1 shows the four roots which satisfy the condition $0 \leq c_i \leq 1$, for $i = 1,5$. Note that they all have monotonically increasing values of c_i. Solution 3 satisfies the constraint that all $b_j > 0$.

Table 1. Four Sets of Coefficients For optimal (5,4) 2N-Storage RK Schemes

COEF	*SOLUTION* 1	*SOLUTION* 2	*SOLUTION* 3	*SOLUTION* 4
A_1	0	0	0	0
A_2	−0.4812317431372	−0.4801594388478	−0.4178904745	−0.7274361725534
A_3	−1.049562606709	−1.4042471952	−1.192151694643	−1.906288083353
A_4	−1.602529574275	−2.016477077503	−1.697784692471	−1.444507585809
A_5	−1.778267193916	−1.056444269767	−1.514183444257	−1.365489400418
B_1	$9.7618354692056E-2$	0.1028639988105	0.1496590219993	$4.1717869324523E-2$
B_2	0.4122532929155	0.7408540575767	0.3792103129999	1.232835518522
B_3	0.4402169639311	0.7426530946684	0.8229550293869	0.5242444514624
B_4	1.426311463224	0.4694937902358	0.6994504559488	0.7212913223969
B_5	0.1978760537318	0.1881733382888	0.1530572479681	0.2570977031703
c_1	0	0	0	0
c_2	$9.7618354692056E-2$	0.1028639988105	0.1496590219993	$4.1717869324523E-2$
c_3	0.3114822768438	0.487989987833	0.3704009573644	0.377744236865
c_4	0.5120100121666	0.6885177231562	0.6222557631345	0.6295990426348
c_5	0.8971360011895	0.9023816453077	0.9582821306748	0.8503409780005

Other values of the parameter α produce similar results, although we have not been able to find roots that satisfy condition III.

The floating point numbers can be expressed as the fractions of integer numbers. For solution 3, the rational form of the coefficients with 26-digit precision becomes

$$A_1 = 0; \quad A_2 = -\frac{567301805773}{1357537059087}; \quad A_3 = -\frac{2404267990393}{2016746695238}; \quad A_4 = -\frac{3550918686646}{2091501179385}; \quad A_5 = -\frac{1275806237668}{842570457699};$$

$$B_1 = \frac{1432997174477}{9575080441755}; \quad B_2 = \frac{5161836677717}{13612068292357}; \quad B_3 = \frac{1720146321549}{2090206949498}; \quad B_4 = \frac{3134564353537}{4481467310338}; \quad B_5 = \frac{2277821191437}{14882151754819};$$

$$c_1 = 0; \quad c_2 = \frac{1432997174477}{9575080441755}; \quad c_3 = \frac{2526269341429}{6820363962896}; \quad c_4 = \frac{2006345519317}{3224310063776}; \quad c_5 = \frac{2802321613138}{2924317926251}$$

and can be used on machines that have up to 26 significant digits without appreciable roundoff errors in the coefficients.

Section 5: Accuracy and Efficiency of (5,4) RK Schemes

The four new (5,4) 2N-storage schemes given in Table 1 are compared with the classical (4,4) 3N-storage RK scheme, the (3,3) 2N-storage RK scheme advocated by Williamson [1] (presented in equation (9)), and the new (4,3) 2N-storage RK scheme presented in equation (10). We begin with a nonlinear ODE used by Dormand et al. [8] to test the accuracy of various RK schemes. The ODE is defined by $y' = y\,cos(x)$, $y(0) = 1$ on the interval $0 \leq x \leq 20$, with the exact solution $y(x) = \exp^{sin(x)}$. Figure 4 shows a convergence study for all seven schemes. The two third-order schemes ((3,3), and (4,3)) approach the exact solution with a slope of -3; the classical fourth-order

(4,4) scheme and the four (5,4) schemes approach the exact solution with a slope of -4. Note that the (3,3) scheme is more accurate than the (4,3) scheme (Williamson claims the (3,3) scheme is optimal in terms of error) and that all (5,4) schemes are more accurate than the (4,4) scheme. Relatively little difference exists between the four (5,4) solutions, and none of the (5,4) schemes is uniformly optimal over the entire range of the refinement study in terms of error.

A second nonlinear test problem is used to establish problem-dependent trends. The ODE is defined by $y' = y\, n\, sin^{n-1}(x) cos(x), \quad y(0) = 1$ on the interval $0 \leq x \leq 20$, with the exact solution $y(x) = \exp^{sin^n(x)}$, where the exponent n is $n = 4$. Figure 5 shows a convergence study for all seven of the schemes. The convergence rates for the 2N-storage schemes are consistent with the theoretical predictions, but the conventional (4,4) scheme converges at a rate that approaches -5. This rate cannot generally be expected. If the four (5,4) 2N-storage schemes are compared between the two nonlinear problems, solution 3 and solution 1 are most accurate in the first and second problems, respectively. No clear advantage is evident for using any particular one of the four (5,4) 2N-storage schemes.

This study verifies the nonlinear accuracy of the newly developed 2N-storage schemes for ODE's. Note that in both test problems, Williamson's (3,3) scheme is more accurate and requires one-third fewer function evaluations than the (4,3) scheme, although no attempt was made to optimize the (4,3) schemes in terms of error. The (5,4) schemes are more accurate than the conventional (4,4) RK scheme in the first problem and more accurate over a significant portion of the second problem. The (5,4) schemes appear to be more adversely affected by roundoff errors than the conventional (4,4) scheme.

Our second problem is the solution of the linear hyperbolic equation defined by

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad 0 \leq x \leq 1, t \geq 0 \tag{14}$$

$$u(0,t) = \sin 2\pi(-t), \quad t \geq 0 \tag{15}$$

$$u(x,0) = \sin 2\pi(x), \quad 0 \leq x \leq 1 \tag{16}$$

The exact solution is

$$u(x,t) = \sin 2\pi(x-t), \quad 0 \leq x \leq 1, t \geq 0$$

and is a model for the class of problems that the (5,4) 2N-storage schemes were developed to integrate.

Equations (14) through (16) are solved with the same four RK schemes used in the nonlinear test problems; specifically, the (3,3) and (4,3) third-order RK schemes and the (4,4) and (5,4) RK schemes. In all cases, the spatial operator used is the sixth-order compact scheme developed by Carpenter et al. [7] and shown to be formally sixth-order accurate. The physical boundary condition is imposed by solving the differentiated boundary condition on the boundary with the RK procedure. This technique was shown by Carpenter et al. [9] to yield a fourth-order temporally accurate procedure. Specifically, the boundary condition is $d^3u(0,t)/dt^3 = g'''(t)$, where g is the physical boundary condition at the inflow plane. The CFL that governs the stability of the hyperbolic problem is a function of the temporal advancement and the spatial discretization used. Table 1 in the appendix compares the inviscid CFL's and the viscous stability limits of the (3,3), (4,4), and (5,4) RK schemes with various spatial operators, including the sixth-order compact spatial operator.

After grid refinement with a vanishingly small CFL, all schemes recover the theoretical spatial sixth-order accuracy. On a specific grid, temporal refinement showed fourth-order temporal accuracy. Table 2 shows the results from a grid-refinement study performed with a CFL of $\frac{3}{2}$ (about $\frac{9}{10}$ of the theoretical maximum CFL) and the (5,4) RK scheme (solution 3).

Table 2. Grid refinement at CFL $= \frac{3}{2}$ for (5,4) 2N-storage RK schemes

Grid	$\log L_2$	Rate
21	-2.4026	
41	-3.3835	3.26
81	-4.5791	3.97
161	-5.7823	4.00
321	-6.9860	4.00
641	-8.1962	4.02

The new scheme is clearly fourth-order accurate for the linear hyperbolic problem. The $\log L_2$ error of all four (5,4) schemes differed in the third significant digit on all grids. In addition, all four schemes were stable up to but not greater than the theoretical stability limit of $CFL_{max} = 1.67$. (See the appendix.)

The relative efficiency of each scheme is not addressed in any of the previously discussed test problems. The advantage in terms of accuracy for the (5,4) schemes is partially lost due to increased function evaluations. To quantify this trade-off, a comparison of accuracy and cost is made between the (3,3), (4,3), (4,4), and (5,4) RK schemes. The test problem is again the hyperbolic wave equation; however, this time the schemes are compared on an equal-cost basis. Here, cost is defined as the number of times the spatial terms are evaluated per unit time interval. The (3,3) RK scheme was run at a CFL of $\frac{3}{k}$, both (4,4) RK schemes were run at a CFL of $\frac{4}{k}$ and the (5,4) RK schemes were run at a CFL of $\frac{5}{k}$, where $4 \le k \le 16$. The resulting schemes are all numerically stable, and temporal errors vary by a factor of 256 for the fourth-order case. The effective cost per unit time was, therefore, identical. All schemes were run to a physical time of $t = 50$. A grid refinement study was also performed to determine the order of accuracy. For all cases, the time asymptotically stable, sixth-order compact spatial operator [7] was used with the boundary conditions that were previously described.

Tables 3(a) and 3(b) show a grid refinement study at two different CFL numbers, the first of which is near the CFL_{max} and the second of which is at half the value of the first. Only the (4,4) RK results are presented here because the (3,4) and the (4,4) RK schemes produce the same results to five significant digits. The results for the (5,4) scheme come from solution 3. (This study is a linear advection problem for which the four-stage third-order scheme performs to fourth-order accuracy.)

Table 3(a). Grid-Refinement Study for Three RK Schemes on Linear Advection Equation $U_t + U_x = 0$, Run at Equal Cost Near Maximum CFL

	(3,3) (2N)		(4,4) (3N)		(5,4) (2N)	
Grid	log L_2	Rate	log L_2	Rate	log L_2	Rate
41	-2.8082		-3.6932		-3.7086	
81	-3.7341	3.08	-4.8877	3.97	-4.8996	3.95
161	-4.6494	2.43	-6.0928	4.00	-6.1039	4.00
321	-5.5567	3.01	-7.2969	4.00	-7.3078	4.00
641	-6.4625	3.01	-8.5054	4.01	-8.5320	4.07

Table 3(b). Grid-Refinement Study for Three RK Schemes on Linear Advection Equation $U_t + U_x = 0$, Run at Equal Cost About Half Maximum CFL

	(3,3) (2N)		(4,4) (3N)		(5,4) (2N)	
Grid	log L_2	Rate	log L_2	Rate	log L_2	Rate
41	-3.6257		-4.2404		-4.2474	
81	-4.6231	3.31	-5.7992	5.18	-5.8032	5.17
161	-5.5515	3.08	-7.2519	4.83	-7.2661	4.85
321	-6.4611	3.02	-8.5021	4.15	-8.5284	4.21
641	-7.3659	3.01	-10.6444	7.11	-9.9965	4.88

The (5,4) and the (4,4) schemes are nearly identical when compared at equal cost. The (5,4) schemes are more susceptible to roundoff errors, as can be identified when the absolute error is near machine precision.

These test problems demonstrate the efficacy of the (5,4) 2N-storage schemes for nonlinear ODE's and the linear PDE's. These results are expected to extend to nonlinear PDE's. If the overriding concern in the choice of integrator is the reduction of storage, then the newly developed (5,4) schemes clearly outperform Williamson's (3,3) 2N-storage scheme in terms of accuracy and efficiency. The accuracy per unit cost is comparable with that of the standard four-stage fourth-order (4,4) RK scheme.

Conclusions

Several new five-stage fourth-order (5,4) Runge-Kutta (RK) schemes are derived that require only two storage locations. Two of the schemes have analytic coefficients that facilitate simple implementation, but neither have desirable stability characteristics. A particular scheme is identified (by numerically solving the nonlinear equations) which has the desirable efficiency characteristics for hyperbolic and parabolic initial (boundary) value problems. In the inviscid and viscous limits, this new (5,4) 2N-storage RK scheme has greater accuracy for a given step size and has a larger allowable stability domain than the (3,3) 2N-storage RK scheme advocated by Williamson. The new (5,4) RK scheme is comparable with the standard (4,4) RK scheme in terms of accuracy to work ratio and is nearly as efficient in an absolute sense. Numerical tests are presented that verify these results on nonlinear ordinary differential equations (ODE's) and linear hyperbolic equations.

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Appendix I

Table A1 shows the inviscid and viscous stability limits obtained from the equation $u_t + au_x = \alpha u_{xx}$, discretized with various spatial and temporal techniques. The inviscid limit is the special case in which $\alpha = 0$; the viscous limit is the special case in which $a = 0$. The first column describes the order of the spatial operator. The letter in parentheses describes the bandwidth of the left-hand-side matrix necessary for compact schemes. Specifically, (E), (T), and (P) signify one-diagonal (explicit), tridiagonal, and pentadiagonal matrices, respectively. The sixth-order (T) is the spatial scheme that is used in all the hyperbolic studies presented in this work. Columns 2-4 report the inviscid stability limits of the (3,3), (4,4), and (5,4) RK schemes, respectively. Columns 5-8 report the viscous stability limits of the (3,3), (4,4), and (5,4) RK schemes, respectively.

For the inviscid case with a sixth-order compact spatial operator (6T), the (3,3) scheme has an effective CFL/stage of $\frac{\sqrt{3}}{6} = 0.289$; the (4,4) and (5,4) schemes are $\frac{\sqrt{2}}{4} = 0.354$ and $\frac{1.67}{5} = 0.334$, respectively. In an absolute sense, the (4,4) RK scheme is the most efficient. Relative to each other, the efficiencies of the (3,3), (4,4), and (5,4) RK schemes are 0.816 : 1.0 : 0.945, respectively, if we assume that the (4,4) scheme has been assigned an efficiency of 1. (Higher numbers are better.)

The viscous CFL/stage for each of the three methods with the (6T) spatial differencing is $\frac{0.630}{3} = 0.210$, $\frac{0.700}{4} = 0.175$, and $\frac{1.17}{5} = 0.234$, respectively. Here, the (5,4) scheme is most efficient, followed by the (3,3) scheme. The relative efficiencies, if we assume that the (4,4) scheme has an absolute efficiency of 1.00, becomes 1.20 : 1.00 : 1.34, respectively, for the (3,3), (4,4) and (5,4) schemes.

For both the inviscid and viscous limits, the (5,4) 2N-storage RK scheme outperforms the (3,3) 2N-storage scheme proposed by Williamson. In the viscous case, the (5,4) scheme dramatically outperforms the conventional (4,4) RK scheme. In the inviscid case, the (5,4) RK scheme is competitive but not quite as efficient as the (4,4) RK scheme.

Table A1: Inviscid and Viscous CFL limits

	Invis	Stab	Limit	Vis	Stab	Limit
Number of stages	3	4	5	3	4	5
Order of accuracy	3	4	4	3	4	4
2nd (E)	$\sqrt{3}$	$2\sqrt{2}$	3.34	2.51	2.78	4.65
4th (E)	1.26	2.06	2.43	1.33	1.47	2.47
4th (T)	1	$\frac{2\sqrt{2}}{\sqrt{3}}$	1.92	0.83	0.92	1.55
6th (E)	1.09	1.78	2.10	0.99	1.10	1.85
6th (T)	$\frac{\sqrt{3}}{2}$	$\sqrt{2}$	1.67	0.63	0.70	1.17
6th (P)	0.88	1.44	1.71	0.65	0.73	1.22
8th (E)	1.00	1.63	1.93	0.83	0.92	1.55
8th (T)	0.81	1.32	1.56	0.55	0.61	1.02
8th (P)	0.78	1.28	1.51	0.51	0.57	0.95
10th (E)	0.94	1.53	1.81	0.74	0.82	1.37
10th (T)	0.77	1.26	1.49	0.50	0.56	0.93
10th (P)	0.74	1.21	1.43	0.46	0.51	0.86
Fourier	$\frac{\sqrt{3}}{\pi}$	$\frac{2\sqrt{2}}{\pi}$	1.07	0.25	0.28	0.47

FIGURE 1. Gross parametric study (in variable α) of stability envelope for RK[5,4] schemes, where $\lambda = \frac{a\Delta t}{\Delta x}$ and $\lambda_v = \frac{\kappa \Delta t}{(\Delta x)^2}$.

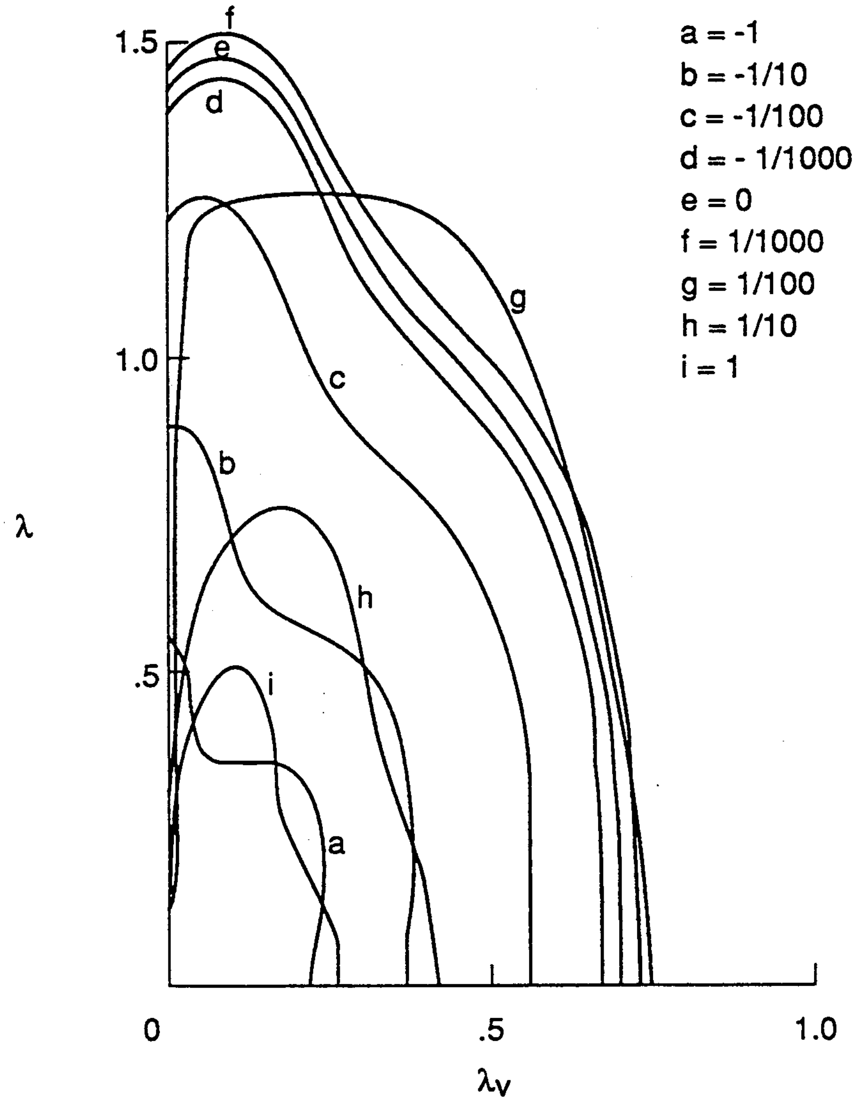


FIGURE 2. Refined parametric study (in variable α) of stability envelope for RK[5,4] schemes.

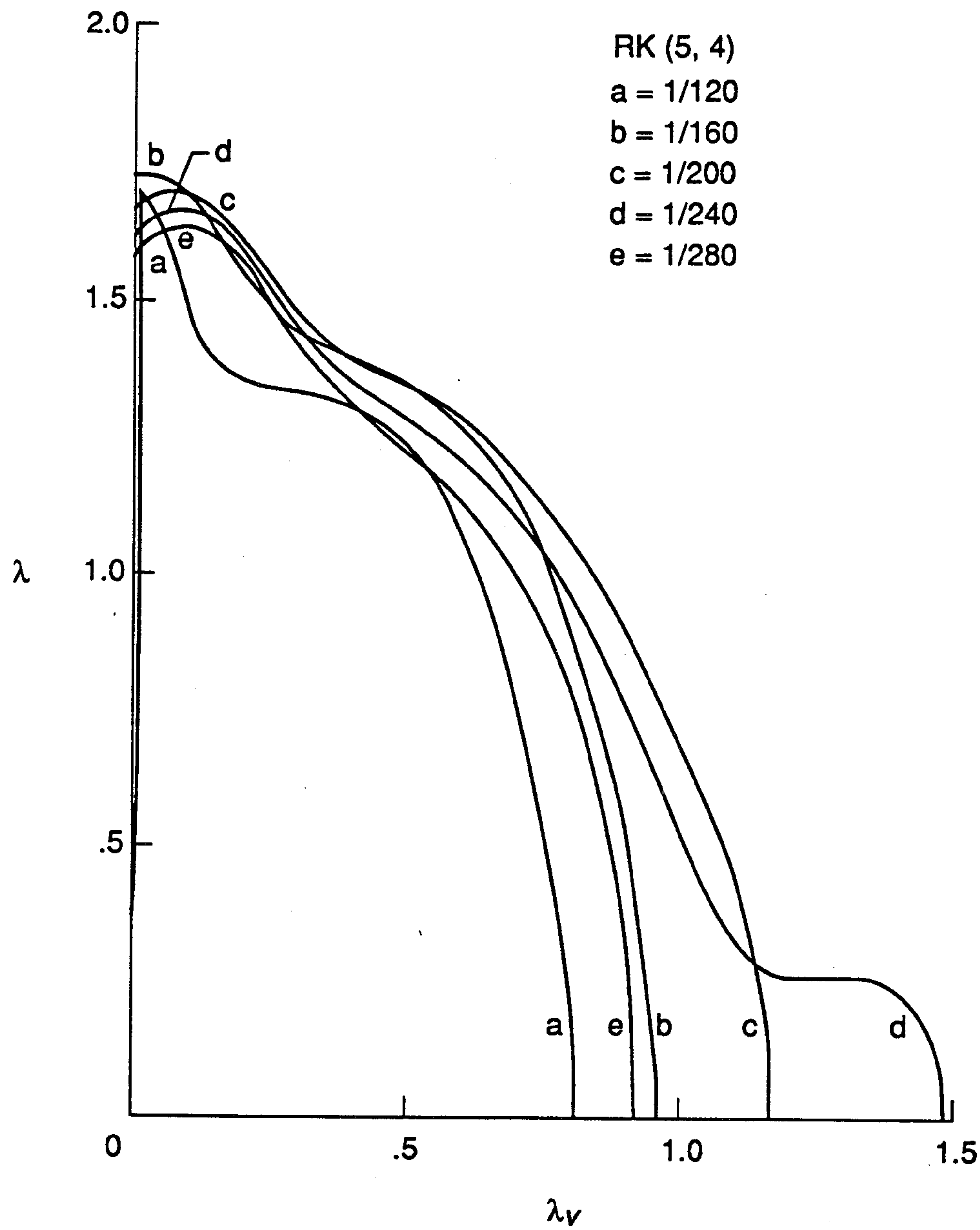


FIGURE 3. Comparison of optimized RK[5,4] schemes with conventional RK[3,3] and RK[4,4] schemes.

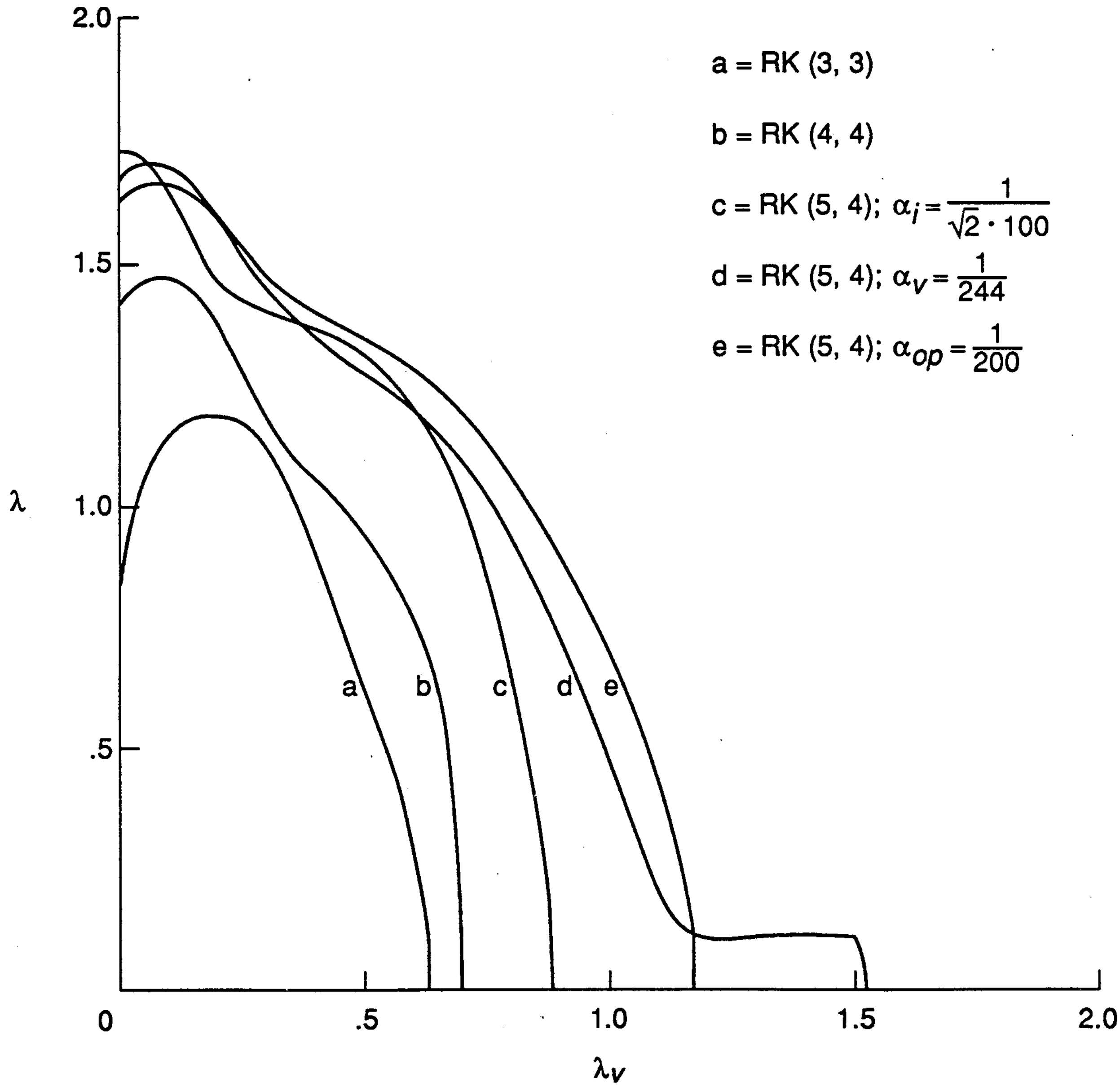


FIGURE 4. Grid convergence study comparing several RK[5,4] schemes with the RK[4,4] and RK[3,3] schemes. Test problem is $y' = y \cos(x)$.

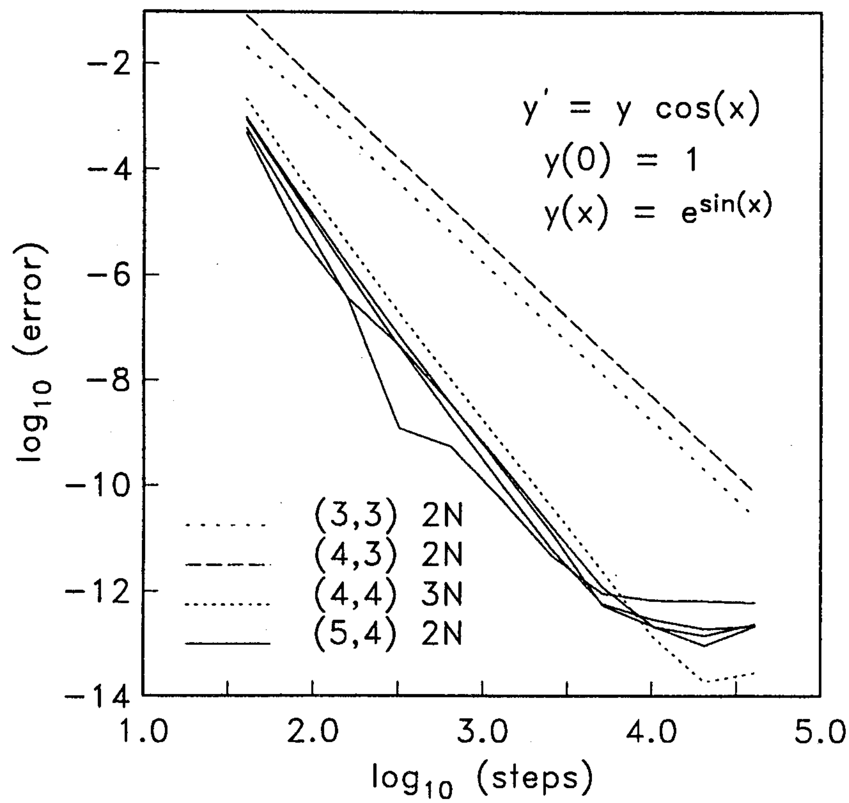
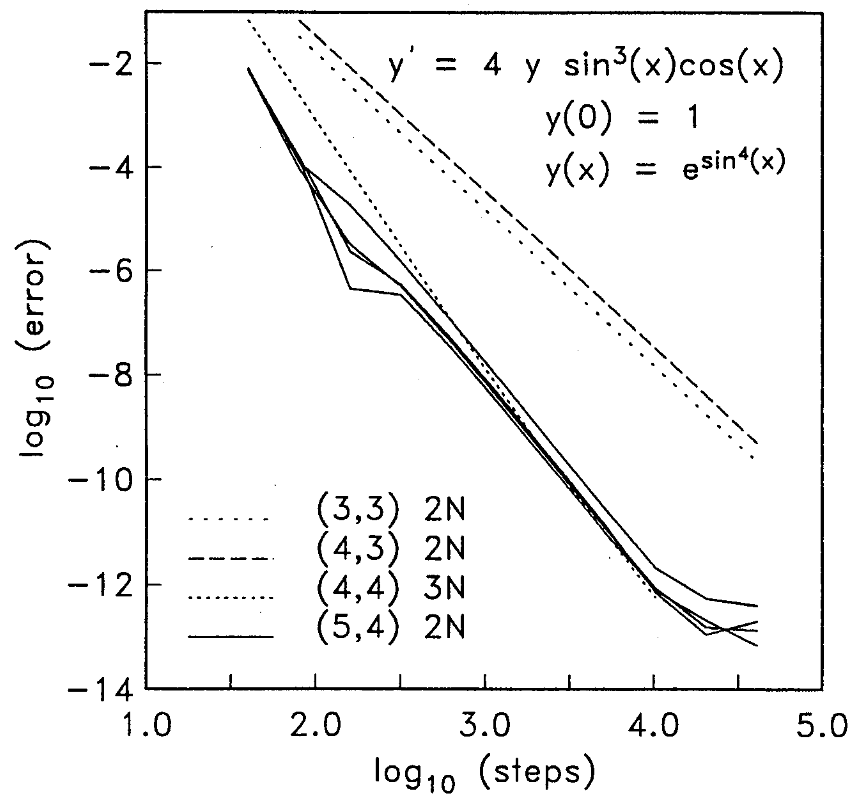


FIGURE 5. Grid convergence study comparing several RK[5,4] schemes with the RK[4,4] and RK[3,3] schemes. Test problem is $y' = 4\,y\,\sin^3(x)\cos(x)$.



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A family of five-stage fourth-order Runge-Kutta schemes is derived; these schemes required only two storage locations. A particular scheme is identified that has desirable efficiency characteristics for hyperbolic and parabolic initial (boundary) value problems. This scheme is competitive with the classical fourth-order method (high-storage) and is considerably more efficient and accurate than existing third-order low-storage schemes.

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