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TWO-STEP RUNGE-KUTTA METHODS*

Z. JACKIEWICZ†‡, R. RENAULT†‡§, AND A. FELDSTEIN†

Abstract. Implicit two-step Runge-Kutta methods are studied. It will be shown that these methods require fewer stages to achieve the same order as one-step Runge-Kutta methods, which means the two-step methods are potentially more efficient than one-step methods. Order conditions are derived and examples of two-step one-stage methods of order 2 and two-step two-stage methods of order 4 are presented. Stability properties of these methods with respect to $y' = ay$ are studied and A -stable two-step methods of order 2 are characterized. Two-step two-stage methods of order 4 which are A -stable are found by an extensive computer search. Semi-implicit two-stage methods of order 4 were also constructed. This is in contrast to the situation encountered in the Runge-Kutta theory where the unique two-stage method of order 4 is not semi-implicit.

Key words. two-step Runge-Kutta method, order conditions, stability analysis

AMS(MOS) subject classifications. 65L05, 65L07

1. Introduction. The purpose of this paper is to study two-step Runge-Kutta (TSRK) methods for the numerical solution of systems of ordinary differential equations (ODEs)

$$(1.1) \quad \begin{aligned} y'(x) &= f(y(x)), & x \in [a, b], \\ y(a) &= y_0, \end{aligned}$$

where the function $f: R^q \rightarrow R^q$ is assumed to be sufficiently smooth. For positive integer N let the stepsize h be given by $h = (b - a)/N$, and define the grid $x_i = a + ih$, $i = 0, 1, \dots, N$. We consider methods of the form

$$(1.2) \quad \begin{aligned} y_{i+1} &= (1 - \theta)y_i + \theta y_{i-1} + h \sum_{j=1}^m (v_j f(Y_{i-1}^j) + w_j f(Y_i^j)), \\ Y_{i-1}^j &= y_{i-1} + h \sum_{s=1}^m a_{js} f(Y_{i-1}^s), & j = 1, 2, \dots, m, \\ Y_i^j &= y_i + h \sum_{s=1}^m a_{js} f(Y_i^s), & j = 1, 2, \dots, m, \end{aligned}$$

$i = 1, 2, \dots, N - 1$. Here, y_i is an approximation to $y(x_i)$, where y is the solution to (1.1), and θ, v_j, w_j , and a_{js} are coefficients of the method. We will represent (1.2) by the following table:

$$\begin{array}{c|c} c & A \\ \hline \theta & v^T \\ & w^T \end{array} = \begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1m} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & \vdots & & \vdots \\ c_m & a_{m1} & a_{m2} & \cdots & a_{mm} \\ \hline \theta & v_1 & v_2 & \cdots & v_m \\ & w_1 & w_2 & \cdots & w_m \end{array},$$

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where $c_i = \sum_{j=1}^m a_{ij}$. Observe that in advancing from t_i to t_{i+1} we need only to compute Y_i^j since Y_{i-1}^j can be taken from the previous step. Therefore we gain extra degrees of freedom associated with a two-step scheme without the need for extra function evaluations.

The special case of these methods corresponding to $\theta = 0$ was first studied by Byrne and Lambert [2]. They considered explicit two-step two-stage and two-step three-stage methods of order 3 and 4, respectively, given by

$$\begin{array}{c|c} 0 & \\ \hline u_1 & u_1 \\ \hline 0 & \begin{array}{cc} A_0 & A_1 \\ B_0 & B_1 \end{array} \end{array} \quad \text{and} \quad \begin{array}{c|cc} 0 & u_1 & \\ \hline u_2 & u_2 - u_3 & u_3 \\ \hline 0 & \begin{array}{ccc} A_0 & A_1 & A_2 \\ B_0 & B_1 & B_2 \end{array} \end{array}.$$

Renaud [10], [11] found methods of the form (1.2) appropriate for the numerical solution of systems of ODEs arising from the semidiscretization of hyperbolic partial differential equations. Verwer [12]–[14] considered two-step and three-step explicit Runge–Kutta methods for the numerical integration of systems resulting from parabolic partial differential equations by applying the method of lines. We refer also to van der Houwen and Sommeijer [7], [8] and van der Houwen [6] for related results concerning explicit k -step m -stage Runge–Kutta methods.

The methods of type (1.2) belong to the class of general linear methods considered by Butcher [1]. Define the vector \tilde{Y}_i

$$\tilde{Y}_i := [Y_i^1, Y_i^2, \dots, Y_i^m, y_{i+1}, y_i]^T,$$

and the $(m+2) \times (m+2)$ matrices \tilde{A} , \tilde{B} , and \tilde{C}

$$\tilde{A} := \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1-\theta & \theta \\ 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix},$$

$$\tilde{B} := \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} & 0 & 0 \\ a_{21} & a_{22} & \cdots & a_{2m} & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mm} & 0 & 0 \\ w_1 & w_2 & \cdots & w_m & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 \end{bmatrix},$$

$$\tilde{C} := \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 \\ v_1 & v_2 & \cdots & v_m & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 \end{bmatrix}.$$

Then the method (1.2) can be written in the form

$$\tilde{Y}_i = (\tilde{A} \otimes I) \tilde{Y}_{i-1} + h(\tilde{B} \otimes I)F(\tilde{Y}_i) + h(\tilde{C} \otimes I)F(\tilde{Y}_{i-1}),$$

where $A \otimes B$ is the direct (tensor) product of matrices A and B , I is the unit $q \times q$ matrix, where q is the dimension of the system (1.1) and

$$F(\tilde{Y}_i) = [f(Y_i^1), f(Y_i^2), \dots, f(Y_i^m), f(y_{i+1}), f(y_i)]^T.$$

The representation of the form $(\tilde{A}, \tilde{B}, \tilde{C})$ is not unique. At the expense of increasing the size of the vector \tilde{Y}_i we could find the standard representation in the form (A^*, B^*) (cf. Butcher [1]). This representation is also not unique.

It is known that the method (1.2) is convergent if and only if it is consistent and zero-stable (see [15]). The method is consistent if it has the order at least 1. This is satisfied if

$$\sum_{j=1}^m (v_j + w_j) = 1 + \theta$$

(cf. § 2). The method is zero-stable if no root of the polynomial

$$\rho(\lambda) = \lambda^2 - (1 - \theta)\lambda - \theta$$

has modulus greater than 1 and if the root has modulus 1 it is simple. This is clearly satisfied if $-1 < \theta \leq 1$.

2. Order conditions. To derive order conditions for the method (1.2) we use the theory by Hairer and Wanner [3]. First, we rewrite (1.2) in the matrix form

$$(2.1) \quad Y = A^{(0)} Y_0 + h A^{(1)} f(Y),$$

where

$$\begin{aligned} Y &= [Y_{i-1}^1, \dots, Y_{i-1}^m, Y_i^1, \dots, Y_i^m, y_{i+1}]^T, \\ Y_0 &= [\underbrace{y_{i-1}, \dots, y_{i-1}}_{m \text{ times}}, \underbrace{y_i, \dots, y_i}_{m+1 \text{ times}}]^T, \\ f(Y) &= [f(Y_{i-1}^1), \dots, f(Y_{i-1}^m), f(Y_i^1), \dots, f(Y_i^m), f(y_{i+1})]^T, \\ A^{(0)} &= \begin{bmatrix} 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ \vdots & & \vdots & \vdots & & & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & \cdots & 0 & \theta & 0 & \cdots & 0 & 1 - \theta & 0 \end{bmatrix}, \\ A^{(1)} &= \begin{bmatrix} a_{11} & \cdots & a_{1m} & 0 & \cdots & 0 & 0 \\ \vdots & & \vdots & \vdots & & \vdots & \vdots \\ a_{m1} & \cdots & a_{mm} & 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & a_{11} & \cdots & a_{1m} & 0 \\ \vdots & & \vdots & \vdots & & \vdots & \vdots \\ 0 & \cdots & 0 & a_{m1} & \cdots & a_{mm} & 0 \\ v_1 & \cdots & v_m & w_1 & \cdots & w_m & 0 \end{bmatrix}. \end{aligned}$$

Observe that $A^{(0)}u = u$, where

$$u = \underbrace{[1, 1, \dots, 1]}_{2m+1 \text{ times}}^T.$$

These definitions of Y , Y_0 , $A^{(0)}$, and $A^{(1)}$ are not unique (see [11] for a slightly different

representation). We also define the $(2m+1)$ -dimensional vector a in such a way that the ν th component of Y_0 is an approximation to the solution $y(x_i + a_\nu h)$ for $\nu = 1, 2, \dots, 2m$, and the $(2m+1)$ st component of Y is computed in order to fit $y(x_i + a_{2m+1}h)$ (cf. [3]). It follows from the form of Y_0 and Y that

$$a = \underbrace{[-1, \dots, -1]}_{m \text{ times}}, \underbrace{[0, \dots, 0]}_{m \text{ times}}, 1]^T.$$

We have the following theorem.

THEOREM 1 (Hairer and Wanner [3]). *The method (2.1) has order s if for all trees t with order $\rho(t) \leq s$, it holds that*

$$(2.2) \quad \phi_{2m+1}(t) = a_{2m+1}^{\rho(t)},$$

where $\phi(t)$ can be computed using the *Kastlunger formula* as follows. For the tree τ consisting only of the root we have

$$(2.3) \quad \phi(\tau) = A^{(0)}a + A^{(1)}u,$$

and if $t = [t_1, t_2, \dots, t_r]$ then

$$(2.4) \quad \begin{aligned} \phi(t) &= A^{(0)}a^{\rho(t)} + A^{(1)}\psi(t), \\ \psi(t) &= \rho(t)\phi(t_1) \cdots \phi(t_r). \end{aligned}$$










Here, $\phi_{2m+1}(t)$ and a_{2m+1} denote the $(2m+1)$ st components of $\phi(t)$ and a , respectively, and $a^{\rho(t)}$ and $\phi(t_1) \cdots \phi(t_r)$ denote componentwise multiplication.

Observe that for our methods $a_{2m+1} = 1$. The order conditions up to order 4 computed by using (2.2)–(2.4) are listed in Table 1, where u denotes the vector $[1, \dots, 1]^T$ of appropriate dimension. These order conditions (in slightly different notation) were obtained before by Renaut [11] using the composition theorem of Hairer and Wanner [4]. In [10] the order conditions were obtained in a more elementary way using the Taylor series expansion.

TABLE 1
Order conditions for TSRK method.

t	$\rho(t)$	Order condition
τ	1	$(v^T + w^T)u = 1 + \theta$
I	$[\tau]$	$2v^T(c - u) + 2w^Tc = 1 - \theta$
V	$[\tau^2]$	$3v^T(c - u)^2 + 3w^Tc^2 = 1 + \theta$
I	$[2\tau]_2$	$6(v^T + w^T)Ac - 6v^Tc + 3v^Tu = 1 + \theta$
V	$[\tau^3]$	$4v^T(c - u)^3 + 4w^Tc^3 = 1 - \theta$
V	$[\tau[\tau]]$	$8(v^T + w^T)(c \cdot Ac) - 4v^T(u - 3c + 2c^2 + 2Ac) = 1 - \theta$
Y	$[2\tau^2]_2$	$12v^TA(c - u)^2 + 12w^TAc^2 - 4v^Tu = 1 - \theta$
I	$[3\tau]_3$	$24(v^T + w^T)A^2c - 24v^TAc + 12v^Tc - 4v^Tu = 1 - \theta$

TABLE 2
Error coefficients for TSRK method of order 4.

t	$\alpha(t)$	$e(t)$
	$[\tau^4]$	1 $1 + \theta - 5v^T(c-u)^4 - 5w^Tc^4$
	$[\tau^2[\tau]]$	6 $1 + \theta - 10v^T(Ac \cdot (c-u)^2) - 10w^T(Ac \cdot c^2) + 10v^T(c \cdot (c-u)^2) - 5v^T(c-u)^2$
	$[\tau[\tau^2]]$	4 $1 + \theta - 15v^T(A(c-u)^2 \cdot c) - 15w^T(Ac^2 \cdot c) + 15v^T A(c-u)^2 + 5v^Tc - 5v^Tu$
	$[\tau[\tau^2]_2]$	4 $1 + \theta - 30(v^T + w^T)(A^2c \cdot c) + 30v^T A^2c + 30v^T(Ac \cdot c) - 30v^TAc - 15v^Tc^2 + 20v^Tc - 5v^Tu$
	$[[\tau]^2]$	3 $1 + \theta - 20(v^T + w^T)(Ac)^2 + 40v^T(Ac \cdot c) - 20v^TAc - 20v^Tc^2 + 20v^Tc - 5v^Tu$
	$[_2\tau^3]_2$	1 $1 + \theta - 20v^T A(c-u)^3 - 20w^TAc^3 - 5v^Tu$
	$[_2\tau[\tau]]_2$	3 $1 + \theta - 40(v^T + w^T)A(Ac \cdot c) + 40v^T A^2c + 40v^TAc^2 - 60v^TAc + 20v^Tc - 5v^Tu$
	$[_3\tau^2]_3$	1 $1 + \theta - 60w^T A^2c^2 - 60v^T A^2(c-u)^2 + 20v^Tc - 5v^Tu$
	$[_4\tau]_4$	1 $1 + \theta - 120(v^T + w^T)A^3c + 120v^T A^2c - 60v^TAc + 20v^Tc - 5v^Tu$

It also follows from [3, Thm. 1] that the local discretization error ℓe of two-step Runge-Kutta method (1.2) of order p is given by

$$\ell e = \frac{h^{p+1}}{(p+1)!} \sum_{\substack{t \in T \\ \rho(t) = p+1}} \alpha(t) e(t) F(t)(y(x_i)) + O(h^{p+2}),$$

$h \rightarrow 0$. Here, $\alpha(t)$ is the number of ways of labelling t with a given totally ordered set V with $\#V = \rho(t)$ (see [1]), $e(t)$ is the error coefficient defined by

$$e(t) = a_{2m+1}^{p+1} - \phi_{2m+1}(t),$$

$a_{2m+1} = 1$, and $F(t)(y(x_i))$ is the elementary differential corresponding to the tree t . The function $\alpha(t)$ and error coefficients $e(t)$ are listed in Table 2 for the method of order 4. The function $\phi(t)$ appearing in $e(t)$ was computed using the Kastlunger formula given in Theorem 1.

3. Stability analysis. In this section we will investigate stability properties of (1.2) with respect to the basic test equation

$$(3.1) \quad y'(x) = ay(x), \quad x \geq 0,$$

where a is a complex parameter. Application of (1.2) to (3.1) leads to

$$(3.2) \quad \begin{aligned} y_{i+1} &= (1 - \theta)y_i + \theta y_{i-1} + \alpha \sum_{j=1}^m (v_j Y_{i-1}^j + w_j Y_i^j), \\ Y_{i-1}^j &= y_{i-1} + \alpha \sum_{s=1}^m a_{js} Y_{i-1}^s, \\ Y_i^j &= y_i + \alpha \sum_{s=1}^m a_{js} Y_i^s, \end{aligned}$$

$i = 1, 2, \dots, N-1$, where $\alpha = ha$. Putting $Y_i = [Y_i^1, Y_i^2, \dots, Y_i^m]^T$, the system (3.2) can be written in the form

$$\begin{aligned}y_{i+1} &= (1 - \theta)y_i + \theta y_{i-1} + \alpha(v^T Y_{i-1} + w^T Y_i), \\Y_{i-1} &= y_{i-1}u + \alpha A Y_{i-1}, \\Y_i &= y_i u + \alpha A Y_i.\end{aligned}$$

Hence,

$$\begin{aligned}Y_{i-1} &= (I - \alpha A)^{-1} u y_{i-1}, \\Y_i &= (I - \alpha A)^{-1} u y_i,\end{aligned}$$

and substituting these expressions into the formula for y_{i+1} we obtain

$$(3.3) \quad y_{i+1} = R(\alpha, \theta)y_i + S(\alpha, \theta)y_{i-1},$$

where

$$(3.4) \quad R(\alpha, \theta) := 1 - \theta + \alpha w^T (I - \alpha A)^{-1} u,$$

$$(3.5) \quad S(\alpha, \theta) := \theta + \alpha v^T (I - \alpha A)^{-1} u.$$

Since uw^T is the matrix of rank 1, the function $R(\alpha, \theta)$ for $\theta \neq 1$ can be written in the form

$$\begin{aligned}R(\alpha, \theta) &= 1 - \theta + \alpha w^T (I - \alpha A)^{-1} u \\&= (1 - \theta) \left[1 + \frac{\alpha}{1 - \theta} w^T (I - \alpha A)^{-1} u \right] \\&= (1 - \theta) \det \left(I + \frac{\alpha}{1 - \theta} (I - \alpha A)^{-1} u w^T \right) \\&= (1 - \theta) \frac{\det (I - \alpha A + (\alpha / (1 - \theta)) u w^T)}{\det (I - \alpha A)},\end{aligned}$$

where the third equality follows from the identity for elementary matrices (see Householder [5, eq. (4), p. 3]). Similarly, for $S(\alpha, \theta)$ and $\theta \neq 0$ we obtain

$$S(\alpha, \theta) = \theta \frac{\det (I - \alpha A + (\alpha / \theta) u v^T)}{\det (I - \alpha A)}.$$

To investigate stability properties of (1.2) with respect to (3.1) we must investigate the asymptotic behaviour of solutions to (3.3). This in turn is determined by the location of roots of the characteristic polynomial

$$(3.6) \quad \phi(\lambda) = \lambda^2 - R(\alpha, \theta)\lambda - S(\alpha, \theta).$$

The stability region of the two-step Runge-Kutta method (1.2) is the set of all points α for which the roots of ϕ are inside or on the unit circle with those on the unit circle being simple. The method is said to be A -stable if its stability region contains the negative half plane. We can determine the stability region of (1.2) by the boundary locus method as follows. Consider the family of equations

$$(3.7) \quad e^{2it} - R(\alpha, \theta) e^{it} - S(\alpha, \theta) = 0,$$

for $t \in [0, 2\pi]$. The solution $\alpha = \alpha(t)$ to (3.7) defines a curve or curves in the complex plane and the boundary of stability region of (1.2) is then, in general, a subset of the union of these curves. We can plot the curve $\alpha = \alpha(t)$, $t \in [0, 2\pi]$, solving (3.7) by, for example, the secant method for $t_k = 2\pi k/M$, $k = 0, 1, \dots, M$, where M is a positive integer. Observe that for $t = 0$ the equation (3.7) takes the form

$$\alpha(v^T + w^T)(I - \alpha A)^{-1}u = 0.$$

Hence, $\alpha(0) = \alpha_0 = 0$ or α_0 is the solution to $(v^T + w^T)(I - \alpha A)^{-1}u = 0$. To compute an approximation α_1 to $\alpha(t_1)$ we can use α_0 and some point close to it as initial guesses. To compute an approximation α_{k+1} to $\alpha(t_{k+1})$, $k = 1, 2, \dots, M-1$, we use α_k and $\alpha_{k-1} + 2(\alpha_k - \alpha_{k-1})$ as initial guesses. Here, α_{k-1} and α_k are approximations to $\alpha(t_{k-1})$ and $\alpha(t_k)$, respectively.

Stability regions obtained in this manner for two-step one-stage methods of order 2 and two-step two-stage methods of order 4 are presented in §§ 4 and 5.

4. Two-step one-stage methods of order 2. Consider the two-step one-stage implicit method of the form

$$\begin{aligned} y_{i+1} &= (1 - \theta)y_i + \theta y_{i-1} + hv_1 f(Y_{i-1}) + hw_1 f(Y_i), \\ (4.1) \quad Y_{i-1} &= y_{i-1} + ha_{11} f(Y_{i-1}), \\ Y_i &= y_i + ha_{11} f(Y_i), \end{aligned}$$

$i = 1, 2, \dots, N-1$. This method has order 2 if the following conditions are satisfied:

$$\begin{aligned} v_1 + w_1 &= 1 + \theta, \\ 2v_1(a_{11} - 1) + 2w_1 a_{11} &= 1 - \theta \end{aligned}$$

(cf. § 2). This system has a two-parameter family of solutions. Choosing θ and a_{11} as free parameters we get

$$\begin{aligned} (4.2) \quad v_1 &= \frac{1}{2}(2a_{11}(1 + \theta) - 1 + \theta), \\ w_1 &= \frac{1}{2}(3 + \theta - 2a_{11}(1 + \theta)). \end{aligned}$$

To investigate whether the method (4.1) can attain order 3 consider the order conditions

$$\begin{aligned} v_1 + w_1 &= 1 + \theta, \\ 2v_1(a_{11} - 1) + 2w_1 a_{11} &= 1 - \theta, \\ 3v_1(a_{11} - 1)^2 + 3w_1 a_{11}^2 &= 1 + \theta, \\ 6(v_1 + w_1)a_{11}^2 - 6v_1 a_{11} + 3v_1 &= 1 + \theta. \end{aligned}$$

Adding the second equation to the third and fourth and subtracting the resulting equations, we obtain

$$3a_{11}^2(v_1 + w_1) = 0.$$

Hence, $a_{11} = 0$ or $v_1 + w_1 = 0$. If $a_{11} = 0$ then $v_1 = 2$, $w_1 = 4$, and $\theta = 5$ and this violates the zero-stability of the method (4.1). On the other hand, if $v_1 + w_1 = 0$ then $v_1 = -1$, $w_1 = 1$, $a_{11} = \frac{1}{2}$, and $\theta = -1$, which again violates the zero-stability of the method (4.1). Therefore, the zero-stable method cannot have order 3.

To investigate stability properties of (4.1) observe that the recurrence relation (3.3) takes the form

$$(4.3) \quad y_{i+1} = \left(1 - \theta + \frac{\alpha w_1}{1 - \alpha a_{11}}\right) y_i + \theta + \frac{\alpha v_1}{1 - \alpha a_{11}}.$$

Solving the equation

$$\lambda^2 - \left(1 - \theta + \frac{\alpha w_1}{1 - \alpha a_{11}}\right) \lambda - \theta - \frac{\alpha v_1}{1 - \alpha a_{11}} = 0$$

with respect to α , we get

$$\alpha = \frac{(\lambda - 1)(\lambda + \theta)}{w_1 \lambda + v_1 + a_{11}(\lambda - 1)(\lambda + \theta)},$$

or by expressing v_1 and w_1 in terms of θ and a_{11} (cf. (4.3)) it follows that

$$\alpha = \frac{2(\lambda^2 - (1 - \theta)\lambda - \theta)}{2a_{11}(\lambda - 1)^2 + (3 + \theta)\lambda - 1 + \theta}.$$

Putting $\lambda = e^{it}$, $t \in [0, 2\pi]$, it follows after straightforward although quite tedious calculations that

$$\begin{aligned} \alpha(t) &= 4(1 - \theta)(2a_{11} - 1)(\cos t - 1)^2 / \Delta \\ &\quad + i(2(2a_{11}(1 + \theta) - 1 + \theta) \sin 2t + 4(2 + \theta + \theta^2 - 2a_{11}(1 + \theta)) \sin t) / \Delta, \end{aligned}$$

where

$$\begin{aligned} \Delta &= (2a_{11} \cos 2t - (4a_{11} - 3 - \theta) \cos t + 2a_{11} - 1 + \theta)^2 \\ &\quad + (2a_{11} \sin 2t - (4a_{11} - 3 - \theta) \sin t)^2 \geq 0. \end{aligned}$$

It follows from the zero-stability of the method (4.1) that $-1 < \theta \leq 1$. Assume first that $-1 < \theta < 1$. In this case it can be checked that if $a_{11} > \frac{1}{2}$ then $\operatorname{Re} \alpha(t) > 0$ for $t \in (0, 2\pi)$. This means that the stability region of (4.1) contains the negative complex plane, or that the method (4.1) is A -stable. If $\theta = 1$ or $a_{11} = \frac{1}{2}$ then $\operatorname{Re} \alpha(t) = 0$ and after some calculations we obtain

$$(4.4) \quad \alpha(t) = i \frac{\sin t}{a_{11} \cos t - a_{11} + 1} \quad \text{if } \theta = 1,$$

or

$$(4.5) \quad \alpha(t) = 2i \tan \frac{t}{2} \quad \text{if } a_{11} = \frac{1}{2}.$$

Observe that (4.4) for $a_{11} = \frac{1}{2}$ reduces to (4.5). It follows from (4.5) that if $a_{11} = \frac{1}{2}$ then the boundary of the stability region of (4.1) is exactly the imaginary axis and this method is A -stable. In particular the method corresponding to $\theta = 1$ and $a_{11} = \frac{1}{2}$ is A -stable in spite of the fact that the polynomial $\rho(\lambda) = (\lambda - 1)(\lambda + 1)$ has both roots on the unit circle. Observe, however, that the characteristic polynomial $\phi(\lambda)$ given by (3.6) in this case takes the form

$$\phi(\lambda) = (\lambda + 1) \left(\lambda - \frac{2 + \alpha}{2 - \alpha} \right).$$

Hence, the solution $\{y_i\}_{i=0}^\infty$ to (4.3) is bounded but does not tend to zero as $i \rightarrow \infty$.

If $\theta = 1$ and $a_{11} = 0$ then it follows from (4.4) that $\alpha = i \sin t$, which means that the region of stability is empty. If $\theta = 1$ and $a_{11} \neq 0$, then

$$\alpha = i \frac{\sin t}{a_{11}(\cos t - (a_{11} - 1)/a_{11})}$$

and the boundary of the stability region is the imaginary axis if and only if $|(a_{11} - 1)/a_{11}| \leq 1$, which gives $a_{11} \geq \frac{1}{2}$.

In the above discussion we have proved the following theorem which characterizes the family of two-step one-stage methods of order 2 that are A-stable.

THEOREM 2. *The two-step one-stage Runge-Kutta method (4.1) with v_1 and w_1 given by (4.2) is A-stable if and only if $-1 < \theta \leq 1$ and $a_{11} \geq \frac{1}{2}$.*

In Fig. 1 stability regions for the method (4.1) with v_1 and w_1 given by (4.2) are presented corresponding to $\theta = \frac{1}{2}$ and $a_{11} = 0, \frac{1}{4}, \frac{3}{4}$, and 1. In the cases $a_{11} = 0$ and $a_{11} = \frac{1}{4}$ the stability regions are just the areas within the curves. In the two plots corresponding to $a_{11} = \frac{3}{4}$ and $a_{11} = 1$ there are two roots of (3.6) greater than 1 inside the inner loops and one root greater than 1 inside the annulus-like regions. Therefore, the stability regions are outside the curves which confirms that A-stability is achieved when $a_{11} \geq \frac{1}{2}$. For $\theta = \frac{1}{2}$ and $a_{11} = \frac{1}{2}$ the stability region is exactly the negative half plane.

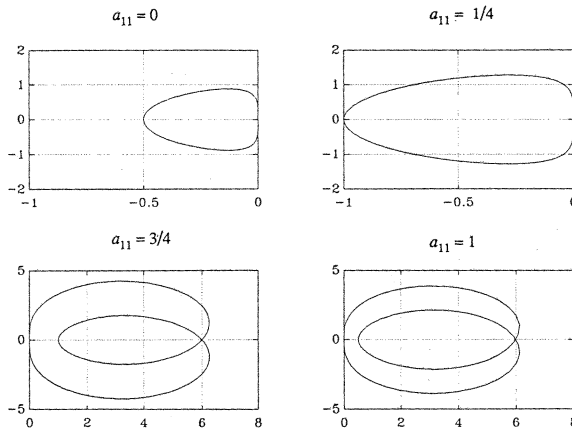


FIG. 1. Stability regions for implicit TSRK methods of order two for $\theta = \frac{1}{2}$.

Two-step Runge-Kutta methods require only one stage to attain order 2. This means that the efficiency of these methods is comparable to that of the implicit midpoint method, backward differentiation formula of order 2, and trapezoidal rule. Since for $a_{11} \geq \frac{1}{2}$ two-step methods are A-stable (cf. Theorem 2), these methods also have stability properties similar to the above-mentioned methods.

5. Two-step two-stage methods of order 4. Consider the two-step two-stage implicit method of the form

$$(5.1) \quad \begin{aligned} y_{i+1} &= (1 - \theta)y_i + \theta y_{i-1} + h \sum_{j=1}^2 (v_j f(Y_{i-1}^j) + w_j f(Y_i^j)), \\ Y_{i-1}^j &= y_{i-1} + h \sum_{s=1}^2 a_{js} f(Y_{i-1}^s), \quad j = 1, 2, \\ Y_i^j &= y_i + h \sum_{s=1}^2 a_{js} f(Y_i^s), \quad j = 1, 2, \end{aligned}$$

$i = 1, 2, \dots, N-1$. For this method order conditions up to order 4 are

$$\begin{aligned}
 \tau: \quad & \sum_i v_i + \sum_i w_i = 1 + \theta, \\
 [\tau]: \quad & 2 \sum_i v_i (c_i - 1) + 2 \sum_i w_i c_i = 1 - \theta, \\
 [\tau^2]: \quad & 3 \sum_i v_i (c_i - 1)^2 + 3 \sum_i w_i c_i^2 = 1 + \theta, \\
 [{}_2\tau]_2: \quad & 6 \sum_{i,j} v_i a_{ij} c_j + 6 \sum_{i,j} w_i a_{ij} c_j - 6 \sum_i v_i c_i + 3 \sum_i v_i = 1 + \theta, \\
 [\tau^3]: \quad & 4 \sum_i v_i (c_i - 1)^3 + 4 \sum_i w_i c_i^3 = 1 - \theta \\
 [\tau[\tau]]: \quad & 8 \sum_{i,j} v_i c_i a_{ij} c_j + 8 \sum_{i,j} w_i c_i a_{ij} c_j - 8 \sum_i v_i a_{ij} c_j \\
 & \quad - 8 \sum_i v_i c_i^2 + 12 \sum_i v_i c_i - 4 \sum_i v_i = 1 - \theta, \\
 [{}_2\tau^2]_2: \quad & 12 \sum_{i,j} v_i a_{ij} (c_j - 1)^2 + 12 \sum_{i,j} w_i a_{ij} c_j^2 - 4 \sum_i v_i = 1 - \theta, \\
 [{}_3\tau]_3: \quad & 24 \sum_{i,j,k} v_i a_{ij} a_{jk} c_k + 24 \sum_{i,j,k} w_i a_{ij} a_{jk} c_k \\
 & \quad - 24 \sum_{i,j} v_i a_{ij} c_j + 12 \sum_i v_i c_i - 4 \sum_i v_i = 1 - \theta.
 \end{aligned}$$

Here and in what follows the summation ranges are from 1 to 2. Observe that if $v_i = 0$ and $\theta = 0$ these conditions reduce to order conditions up to order 4 for Runge-Kutta methods (cf. [1]).

We will not try to solve the above system in full generality but impose some simplifying conditions. Assume first that

$$(5.2) \quad \sum_j a_{ij} c_j = \frac{1}{2} c_i^2, \quad i = 1, 2,$$

which are the familiar row simplifying conditions appearing in the theory of Runge-Kutta methods. Then it can be checked that the order conditions corresponding to $[\tau^2]$, $[{}_2\tau^2]_2$, and $[\tau^3]$ are the same as those corresponding to $[{}_2\tau]_2$, $[{}_3\tau]_3$, and $[\tau[\tau]]$, respectively. The remaining five order conditions take the form

$$\begin{aligned}
 (5.3) \quad & \sum_i v_i + \sum_i w_i = 1 + \theta, \\
 & \sum_i v_i (c_i - 1) + \sum_i w_i c_i = \frac{1 - \theta}{2}, \\
 & \sum_i v_i (c_i - 1)^2 + \sum_i w_i c_i^2 = \frac{1 + \theta}{3}, \\
 & \sum_i v_i (c_i - 1)^3 + \sum_i w_i c_i^3 = \frac{1 - \theta}{4},
 \end{aligned}$$

and

$$(5.4) \quad 12 \sum_{i,j} v_i a_{ij} (c_j - 1)^2 + 12 \sum_{i,j} w_i a_{ij} c_j^2 - 4 \sum_i v_i = 1 - \theta.$$

Eliminating θ from (5.3) and (5.4) we obtain

$$\begin{aligned}\sum_i v_i \left(3 \sum_j a_{ij} c_j^2 - c_i^3 \right) + \sum_i w_i \left(3 \sum_j a_{ij} c_j^2 - c_i^3 \right) &= 0, \\ \sum_i v_i (2c_i^3 - 6c_i^2 + 5c_i - 1) + \sum_i w_i (2c_i^3 - c_i) &= 0, \\ \sum_i v_i (3c_i^2 - 6c_i + 2) + \sum_i w_i (3c_i^2 - 1) &= 0, \\ \sum_i v_i (2c_i - 1) + \sum_i w_i (2c_i + 1) &= 2.\end{aligned}$$

We have also $\sum_j a_{ij} = c_i$, $i = 1, 2$ (compare § 1) and (5.2), which for $c_1 \neq c_2$ lead to the following formulae for a_{ij} , $i, j = 1, 2$:

$$\begin{aligned}a_{11} &= \frac{c_1(2c_2 - c_1)}{2(c_2 - c_1)}, & a_{12} &= -\frac{c_1^2}{(2(c_2 - c_1))}, \\ a_{21} &= \frac{c_2^2}{2(c_2 - c_1)}, & a_{22} &= \frac{c_2(c_2 - 2c_1)}{2(c_2 - c_1)}.\end{aligned}$$

It can also be checked that when $c_1 \rightarrow c_2$ then $\theta \rightarrow -1$ and in the limit the condition of zero-stability is violated.

We have performed an extensive computer search looking for A -stable TSRK methods with minimal normalized error constant defined by

$$G(c_1, c_2) := \max \{ |e(t)| : t \in T, \rho(t) = 5 \} / |1 + \theta|$$

(cf. [10], [12]). Observe first that if the two-step Runge-Kutta method has the form

$$\begin{array}{c|c} c & A \\ \hline \theta & \begin{array}{c} v^T \\ w^T \end{array} \end{array} = \begin{array}{c|c} c_1 & \begin{array}{cc} a_{11} & a_{12} \end{array} \\ c_2 & \begin{array}{cc} a_{21} & a_{22} \end{array} \\ \hline \theta & \begin{array}{cc} v_1 & v_2 \\ w_1 & w_2 \end{array} \end{array},$$

then interchanging c_1 and c_2 leads to the new method of the form

$$\begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline \tilde{\theta} & \begin{array}{c} \tilde{v}^T \\ \tilde{w}^T \end{array} \end{array} = \begin{array}{c|c} c_2 & \begin{array}{cc} a_{22} & a_{21} \end{array} \\ c_1 & \begin{array}{cc} a_{12} & a_{11} \end{array} \\ \hline \theta & \begin{array}{cc} v_2 & v_1 \\ w_2 & w_1 \end{array} \end{array}$$

with $\tilde{c} = Pc$, $\tilde{A} = PAP$, $\tilde{v} = Pv$, and $\tilde{w} = Pw$, where P is the permutation matrix $P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. We have $\tilde{\theta} = \theta$ and

$$\begin{aligned}\tilde{R}(\alpha, \tilde{\theta}) &= 1 - \tilde{\theta} + \alpha \tilde{w}^T (I - \alpha \tilde{A})^{-1} u \\ &= 1 - \theta + \alpha w^T P (I - \alpha PAP)^{-1} u \\ &= 1 - \theta + \alpha w^T (I - \alpha A)^{-1} u = R(\alpha, \theta).\end{aligned}$$

Similarly, $\tilde{S}(\alpha, \tilde{\theta}) = S(\alpha, \theta)$ and it follows that both methods have identical stability properties with respect to the test equation (3.1). Moreover, it is easy to check that both methods have identical error coefficients $e(t)$ listed in Table 2. Therefore we can restrict the computer search to the subset $\{(c_1, c_2) : c_1 > c_2\}$ of the $c_1 - c_2$ plane.

The results of this search are presented in Fig. 2 for $0 \leq c_1 \leq 2$ and $0 \leq c_2 < c_1$. The region of A -stability extends to the right of $c_1 = 2$ and the magnified region is presented in Fig. 3 for $1 \leq c_1 \leq 4$ and $0.25 \leq c_2 \leq 0.50$, where we have used the symbol “+” to denote A -stable methods for which $\theta \in (-1, -0.9]$. In Fig. 4 the graphs of the normalized error constant $G(c_1, c_2)$ are presented for $0.5 \leq c_1 \leq 3$ and $c_2 = \frac{103}{256}$. This graph, as well as the others not presented here, indicates that the A -stable two-step Runge-Kutta methods of order 4 with the smallest normalized error constant $G(c_1, c_2)$ correspond to the methods with smallest possible parameter c_1 . We have found experimentally

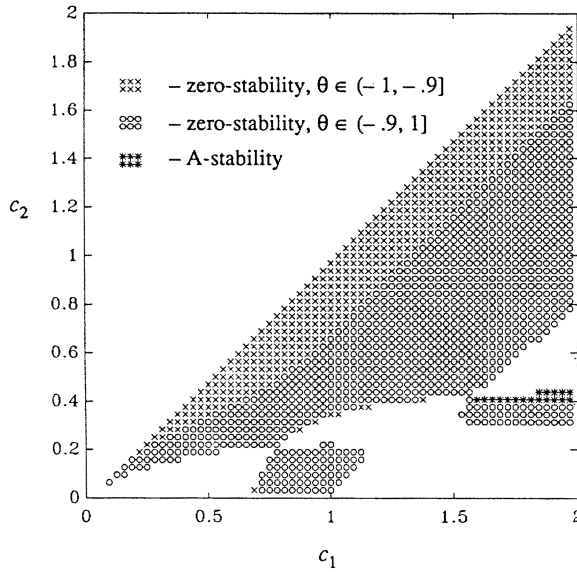


FIG. 2. Region of zero-stability and A -stability in $c_1 - c_2$ plane of implicit TSRK methods of order 4.

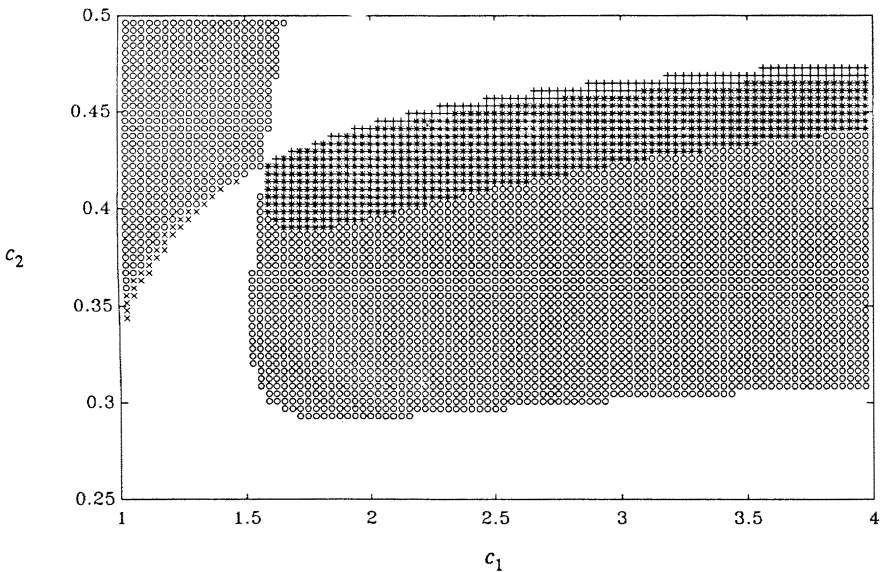


FIG. 3. Region of zero-stability and A -stability in $c_1 - c_2$ plane of implicit TSRK methods of order 4.

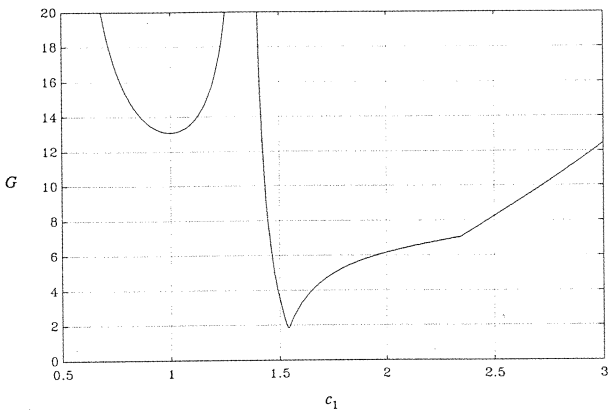


FIG. 4. Normalized error constant $G(c_1, c_2)$ for implicit TSRK methods of order 4 for $c_2 = \frac{103}{256}$.

that the method presented below:

$\frac{51}{32}$	$\frac{5151}{9760}$	$\frac{2601}{2440}$
$\frac{103}{256}$	$\frac{10609}{156160}$	$\frac{73439}{156160}$
$\frac{16977449}{36697976}$	$\frac{636886846889}{1074516737280}$	$\frac{61448158637}{134314592160}$
	$\frac{21872982199}{1074516737280}$	$\frac{52658918227}{134314592160}$

is close to optimal, its normalized error constant is $G(c_1, c_2) \approx 3.09$. The region of absolute stability of this method is presented in Fig. 5. The stability region is outside the solid curve. In the region between the solid curve and the dashed curve the modulus of one root of (3.6) is less than 1 and the modulus of the other root is greater than 1. The moduli of both roots are greater than 1 inside the dotted curve. We have also

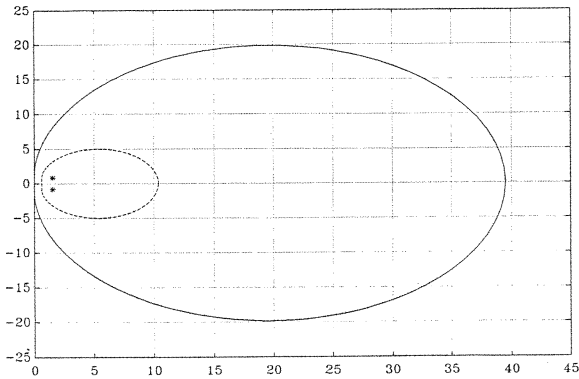


FIG. 5. Region of absolute stability of implicit TSRK methods of order 4 for $c = [\frac{51}{32}, \frac{103}{256}]^T$.

denoted by an asterisk “*” the (common) poles of the stability functions $R(\alpha, \theta)$ and $S(\alpha, \theta)$, i.e., the roots of the equation

$$\det(I - \alpha A) = \det(A)\alpha^2 - \operatorname{tr}(A)\alpha + 1 = 0.$$

These curves were obtained using the boundary locus method described in § 3. For the method (5.1) the solution to the equation

$$\alpha(v^T + w^T)(I - \alpha A)^{-1}u = 0$$

is $\alpha = 0$ and

$$\alpha = \frac{1 + \theta}{(v_1 + w_1)(a_{22} - a_{12}) + (v_2 + w_2)(a_{11} - a_{21})}.$$

It is clear that the method cannot be A -stable if α given by the last formula is less than zero and this fact was used to increase the efficiency of the computer search described above. This computer search was performed using PRO-MATLAB on an Ardent Titan computer at the computer center of the Department of Mathematics, Arizona State University.

6. Semi-implicit two-step two-stage methods of order 4. In this section we will try to construct semi-implicit TSRK methods (5.1), i.e., methods for which $a_{12} = 0$. In this case $c_1 = a_{11}$ and the order conditions take the form

$$\tau: \quad v_1 + w_1 + v_2 + w_2 = 1 + \theta,$$

$$[\tau]: \quad v_1(a_{11} - 1) + v_2(c_2 - 1) + w_1a_{11} + w_2c_2 = \frac{1 - \theta}{2},$$

$$[\tau^2]: \quad v_1(a_{11} - 1)^2 + v_2(c_2 - 1)^2 + w_1a_{11}^2 + w_2c_2^2 = \frac{1 + \theta}{3},$$

$$[{}_2\tau]_2: \quad 2(v_1 + w_1)a_{11}^2 + 2(v_2 + w_2)(a_{21}a_{11} + a_{22}c_2) - 2v_1a_{11} \\ - 2v_2c_2 + v_1 + v_2 = \frac{1 + \theta}{3},$$

$$[\tau_3]: \quad v_1(a_{11} - 1)^3 + v_2(c_2 - 1)^3 + w_1a_{11}^3 + w_2c_2^3 = \frac{1 - \theta}{4},$$

$$[\tau[\tau]]: \quad 2(v_1 + w_1)a_{11}^3 + 2(v_2 + w_2)(a_{21}a_{11} + a_{22}c_2) - v_1(1 - 3a_{11} + 4a_{11}^2) \\ - v_2(1 - 3c_2 + 2c_2^2 + 2a_{21}a_{11} + 2a_{22}c_2) = \frac{1 - \theta}{4},$$

$$[{}_2\tau^2]_2: \quad 3v_1a_{11}(a_{11} - 1)^2 + 3v_2(a_{21}(a_{11} - 1)^2 + a_{22}(c_2 - 1)^2) + 3w_1a_{11}^3 \\ + 3w_2(a_{21}a_{11}^2 + a_{22}c_2^2) - v_1 - v_2 = \frac{1 - \theta}{4},$$

$$[{}_3\tau]_3: \quad 6(v_1 + w_1)a_{11}^3 + 6(v_2 + w_2)(a_{11}a_{21}(a_{11} + a_{22}) + a_{22}^2c_2) \\ - 6v_1a_{11}^2 - 6v_2(a_{11}a_{21} + a_{22}c_2) + 3v_1a_{11} + 3v_2c_2 - v_1 - v_2 = \frac{1 - \theta}{4}.$$

Subtracting the order condition corresponding to $[{}_2\tau]_2$ from that corresponding to $[\tau^2]$ we get

$$(6.1) \quad (v_1 + w_1)a_{11}^2 + (v_2 + w_2)(2a_{11}a_{21} + a_{22}^2 - a_{21}^2) = 0.$$

Subtracting the equation corresponding to $[\tau^3]$ from the equations corresponding to $[\tau[\tau]]$, $[_2\tau^2]_2$, and $[_3\tau]_3$ we obtain

$$(6.2) \quad \begin{aligned} & (v_1 + w_1)a_{11}^3 + (v_2 + w_2)(a_{21} + a_{22})(2a_{11}a_{21} + a_{22}^2 - a_{21}^2) \\ & - v_1a_{11}^2 - v_2(2a_{11}a_{21} + a_{22}^2 - a_{21}^2) = 0, \end{aligned}$$

$$(6.3) \quad \begin{aligned} & 2(v_1 + w_1)a_{11}^3 + (v_2 + w_2)(3a_{21}a_{11}^2 + (a_{21} + a_{22})^2(2a_{22} - a_{21})) \\ & - 3(v_1a_{11}^2 + v_2(2a_{11}a_{21} + a_{22}^2 - a_{21}^2)) = 0, \end{aligned}$$

and

$$(6.4) \quad \begin{aligned} & 5(v_1 + w_1)a_{11}^3 + (v_2 + w_2)(6a_{11}a_{21}(a_{11} + a_{22}) \\ & + (a_{21} + a_{22})(5a_{22}^2 - 2a_{21}a_{22} - a_{21}^2)) \\ & - 3(v_1a_{11}^2 + v_2(2a_{11}a_{21} + a_{22}^2 - a_{21}^2)) = 0. \end{aligned}$$

Subtracting (6.3) from (6.4) and three times (6.2) from (6.4) yields

$$(6.5) \quad \begin{aligned} & (v_1 + w_1)a_{11}^3 + (v_2 + w_2)(a_{22}(a_{21} + a_{22})(a_{22} - a_{21}) \\ & + a_{11}a_{21}(a_{11} + 2a_{22})) = 0, \end{aligned}$$

and

$$(6.6) \quad \begin{aligned} & (v_1 + w_1)a_{11}^3 + (v_2 + w_2)(3a_{11}a_{21}(a_{11} + a_{22}) \\ & + (a_{21} + a_{22})(a_{22}^2 + a_{21}^2 - a_{21}a_{22} - 3a_{11}a_{21})) = 0. \end{aligned}$$

Finally, subtracting (6.5) from (6.6) we obtain

$$a_{21}(a_{21} - 2a_{11})(a_{21} + a_{22} - a_{11})(v_2 + w_2) = 0.$$

It can be checked that there are no zero-stable semi-implicit methods if $a_{21} = 0$ or $a_{21} - 2a_{11} = 0$ or $a_{21} + a_{22} - a_{11} = 0$. If $v_2 + w_2 = 0$, then by (6.1), $v_1 + w_1 = 0$ or $a_{11} = 0$. There are no zero-stable semi-implicit methods if $v_1 + w_1 = 0$ and assuming $a_{11} = 0$ we obtain the following one-parameter family of methods:

0	0	0
4	2	2
$\frac{4}{5-\theta}$	$\frac{2}{5-\theta}$	$\frac{2}{5-\theta}$
θ	$\frac{\theta-1}{2} + \frac{(\theta-5)^2}{48}$	$-\frac{(\theta-5)^2}{48}$
θ	$\frac{3+\theta}{2} - \frac{(\theta-5)^2}{48}$	$\frac{(\theta-5)^2}{48}$

where $-1 < \theta \leq 1$. Observe that this is in contrast to the situation we encounter in the theory of Runge-Kutta methods where the unique two-stage Runge-Kutta method of order 4 is not semi-implicit (cf. [1]).

The semi-implicit method (6.7) cannot be A -stable for any $\theta \in (-1, 1]$. This can be easily seen from the following argument. The TSRK method is A -stable if

$$\phi(\lambda) = \lambda^2 - R(\alpha, \theta)\lambda - S(\alpha, \theta),$$

where $R(\alpha, \theta)$ and $S(\alpha, \theta)$ are defined by (3.4) and (3.5), is a Schur polynomial for all $\alpha \in C^- := \{\alpha: \operatorname{Re}(\alpha) < 0\}$. By the Schur criterion a necessary condition for this is that $|S(\alpha, \theta)| < 1$ for all $\alpha \in C^-$. For the method (6.7) this inequality takes the form

$$\left| \theta + \frac{\theta^2 - 2\theta + 5}{2(\theta - 5)} \alpha + \frac{\theta^2 + 2\theta + 13}{12(\theta - 5)} \alpha^2 \right| < \left| 1 + \frac{2}{\theta - 5} \alpha \right|.$$

Since $\theta^2 + 2\theta + 13 > 0$ for all θ this inequality cannot be satisfied for all $\alpha \in C^-$ for any $\theta \in (-1, 1]$.

Denote by $(\beta(\theta), 0)$ the interval of absolute stability of the semi-implicit method (6.7). The function $\beta(\theta)$, which was computed by bisection method, is plotted in Fig. 6. This function changes slowly, approximately linearly, as θ ranges from -1 to $\theta_0 \approx -0.25$ and then quite rapidly as θ ranges from θ_0 to zero. We have also plotted in Fig. 7 the normalized error constant of the method (6.7) defined by

$$G(\theta) := \max \{ |e(t)| : t \in T, \rho(t) = 5 \} / |1 + \theta|.$$

This error constant decreases rapidly as θ ranges from -1 to approximately -0.5 and then decreases slowly as θ ranges from -0.5 to 1 . There is a tradeoff between the stability and error properties of semi-implicit methods (6.7) and by inspecting Figs. 6 and 7 it follows that the values of θ between -0.35 and -0.25 seem to be optimal. They correspond to the methods with relatively large interval of absolute stability and normalized error constant of moderate size.

Although we have shown that the two-stage fourth-order semi-implicit methods cannot be A -stable, this result does not demonstrate that this method is not efficient for nonstiff problems. Consider, for example, the four-stage, fourth-order, one-step

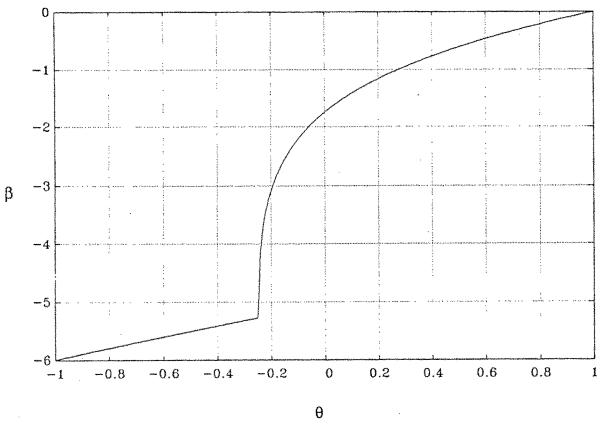


FIG. 6. Function $\beta = \beta(\theta)$ for semi-implicit TSRK methods of order 4.

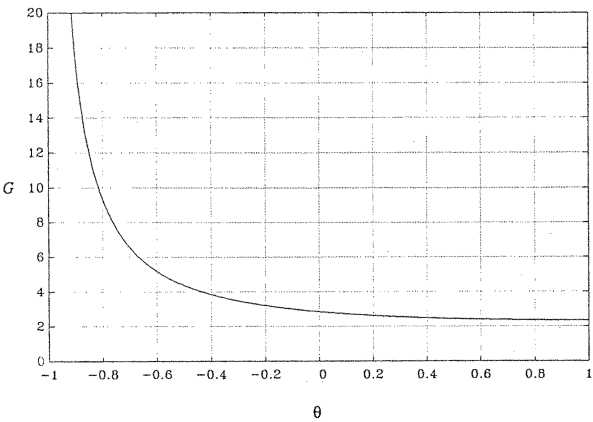


FIG. 7. Normalized error constant $G(\theta)$ for semi-implicit TSRK methods of order 4.

explicit method. The truncation coefficients of this method are about the same size as those of the two-step method, while its interval of absolute stability is about one-half that of the optimal two-step method. The latter comparison means that we should regard the one-step method as requiring eight derivative evaluations to advance a step. Whether or not the two-step method costs more than this depends on the number of implicit stages to be solved and how many iterations are required to convergence. But from (6.7) we observe that only the calculation of $f(Y_i^2)$ is implicit, the value of $f(Y_{i-1}^2)$ already existing from the previous step.

To evaluate the relative efficiency of the method (6.7) we tested it on a few examples. We compared, using as an initial estimate of the stage values, (a) $f(Y_i^2) = f(Y_{i-1}^2)$ and (b) $f(Y_i^2) = 0$. Although both choices gave good convergence, choice (a) was marginally more efficient. In each case, we iterated to convergence until two successive approximations differed by less than h^5 , which is proportional to the local truncation error of the fourth-order method. Observe that the minimum number of derivative evaluations to advance a step is just 2. For low precision we found that the average number of derivative evaluations to advance a step was also near 2. As the accuracy demanded is increased, this number increases slowly to around 4 for an accuracy of about 10^{-9} . Hence the two-step method is between two and four times more efficient than the one-step method. Varying c_1 and c_2 which amounts to varying θ hardly affected the cost of the method. We observed that as θ increased through the range $[-1, 1]$ the number of iterations required, in most cases, increased only slightly. With one exception, this increase was more pronounced at high precisions than low precisions. In this latter case, as θ increased through positive values, convergence was only achieved, if at all, after many iterations. For higher precision, convergence was achieved and the order of the method maintained.

Next we will investigate whether the semi-implicit Runge-Kutta method of order 3 can be embedded into (6.7). Order 3 Runge-Kutta methods of this type take the form

$$(6.8) \quad \begin{array}{c|cc} c_1 & c_1 & 0 \\ \hline \frac{1}{2} + \frac{1}{12} & \frac{1}{6} & \frac{1}{6} - \frac{1}{2}c_1 \\ \frac{2}{2} + \frac{1}{2} - c_1 & \frac{1}{2} - c_1 & \frac{1}{2} - c_1 \\ \hline & \frac{1}{12} & \frac{(\frac{1}{2} - c_1)^2}{c_1^2 - c_1 + \frac{1}{3}} \\ & c_1^2 - c_1 + \frac{1}{3} & c_1^2 - c_1 + \frac{1}{3} \end{array}$$

(cf. [1]). Comparing (6.7) and (6.8), it follows that these methods can form an embedded pair only if $c_1 = 0$ and $\theta = -1$, which violates the zero-stability of the method (6.7). However, embedded pairs of explicit continuous Runge-Kutta methods of order $p-1$ and explicit TSRK methods of order p for $p = 2, 3, 4$, and 5 , were constructed recently by Jackiewicz and Zennaro [9].

7. Concluding remarks. In this paper we have studied the class of two-step Runge-Kutta methods for the numerical solution of ordinary differential equations. The order conditions and the formula for the principal part of the local discretization error are derived using the theory of Hairer and Wanner and the Kastlunger formula. These order conditions are listed up to order 4 (Table 1) along with error coefficients corresponding to the trees of order 5 (Table 2). A stability analysis with respect to the test equation $y' = ay$, where a is a complex parameter, of two-step one-stage methods of order 2 is presented and A-stable methods are characterized. For the solution of systems of ODEs arising from the semidiscretization of partial differential equations of parabolic type stability regions which extend far along the negative real axis are

required (see [12]–[14]). Thus A -stable methods may be useful in this context. Furthermore, the semidiscretization of hyperbolic partial differential equations leads to a requirement of stability along the imaginary axis or in a region in the left half plane (see [10], [11]), and A -stable methods may again be useful. Two-step two-stage methods of order 4 are also studied. An extensive computer search was performed to find the methods which are A -stable and the region of A -stability was presented as a plot in $c_1 - c_2$ plane. We investigated how much the normalized error constant varies across the region of A -stability and give an example of an A -stable method with a small error constant. Next, semi-implicit methods of order 4 are studied. These methods are not A -stable but have quite large interval of absolute stability for $\theta \in (-1, \theta_0)$, where $\theta_0 \approx -0.25$. The normalized error constant tends to infinity as $\theta \rightarrow -1$; however, for θ between approximately -0.35 and -0.25 the error constant is of moderate size and at the same time these methods have a relatively large interval of absolute stability. Numerical tests indicate that these methods are between two and four times more efficient than the one-step fourth-order four-stage explicit Runge–Kutta methods.

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