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EFFICIENTLY IMPLEMENTABLE ALGEBRAICALLY STABLE RUNGE–KUTTA METHODS*

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Abstract. Recent work by Butcher [BIT, 16 (1976), pp. 237–240] on the implementation of implicit Runge–Kutta methods has shown that, if his technique is used, the most efficiently implementable methods are those whose Runge–Kutta matrix has a single real eigenvalue. In this paper, therefore, we analyze the algebraic stability of two families of methods with this property, namely singly-implicit and diagonally implicit methods.

1. Introduction. Recently a number of authors, in particular Nørsett [12], Alexander [1], Butcher [9], Bickart [2] and Varah [14], have shown that implicit Runge–Kutta methods can be implemented much more efficiently than was previously thought possible. In this paper we will focus our attention on the paper of Butcher [9], in which he shows that the most efficient methods when using his implementation are those whose Runge–Kutta matrix has a single real eigenvalue. Two classes of methods have been proposed which possess this property, namely, singly-implicit methods (see Burrage [4]) and diagonally implicit methods (see Nørsett [12] and Alexander [1]). However, although the A-stability of these two classes of methods has already been studied [4], [12] and [1], recent work by Burrage and Butcher [6] suggests that it is not sufficient merely to study the A-stability of a particular method but that its algebraic stability should also be studied. Thus in this paper we will examine the algebraic stability properties of singly-implicit and diagonally-implicit methods.

Before we study the stability properties of these methods, however, the following definitions and results on the order of Runge–Kutta methods will be found useful. As in Butcher [7], we define the following relationships on the coefficients a_{ij}, internal abscissae c_i, and weights b_i:

$$C(p):\quad \sum_{j=1}^{s} a_{ij}c_j^{k-1} = c_i^k/k \text{ for } i=1,\cdots,s \text{ and } k\leqq p,$$

$$D(p):\quad \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} = b_j(1-c_j^k)/k \text{ for } j=1,\cdots,s \text{ and } k\leqq p,$$

$$B(p):\quad g_k=0 \text{ for } k=1,\cdots,p,$$

where $(1+g_k)/k=\sum_{i=1}^{s} b_i c_i^{k-1}$ for $k=1,\cdots,2s$.

For an s-stage Runge–Kutta method, Butcher [7] has proved the following sufficient (but not necessary) result for a method to be of order p.

LEMMA 1. *$C(\eta), D(\xi), B(p)$, where $p\leqq \xi+\eta+1$, $p\leqq 2\eta+2$ implies that a method is of order p.*

Burrage [4] originally defined a Runge–Kutta method to be singly-implicit if the Runge–Kutta matrix has one real s-fold eigenvalue, and the internal abscissae $c_1,\cdots,c_s$ are distinct and satisfy $C(s-1)$, so that if $B(s)$ also holds the method is of order s. This definition has now been widened by most authors so that a singly-implicit method is any method whose Runge–Kutta matrix has a single real s-fold eigenvalue, while a DIRK (diagonally implicit Runge–Kutta method) is a singly-implicit method

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whose Runge–Kutta matrix is lower triangular. In this paper we will use the more general definition of singly-implicitness. In § 2 we will derive some results on the algebraic stability properties of Runge–Kutta methods and show that an algebraically stable DIRK cannot have order more than 4. In § 3 we will construct algebraically stable singly-implicit methods of orders 1, 2, 3 and 4, while in § 4 we will construct the complete family of s-stage algebraically stable DIRK's of order s ($s \leqq 4$).

2. Some general results. This paper is concerned with the study of the nonlinear stability properties of two special classes of implicit Runge–Kutta methods. The stability property in question is called B-stability, and was introduced by Butcher [8]. It is based on the general test equation $y'(x) = f(y(x))$, $f: \mathbb{R}^N \to \mathbb{R}^N$, where $\langle f(u) - f(v), u - v\rangle \leqq 0$ for all u, $v \in \mathbb{R}^N$, and is more suited to modeling nonlinear equations than is the weaker property of A-stability. A sufficient condition for B-stability (called algebraic stability) has been derived by Burrage and Butcher [6], requiring the weights $b_1, \cdots, b_s \geqq 0$ and the stability matrix M (whose (i, j) element is $b_i a_{ij} + b_j a_{ji} - b_i b_j$) to be nonnegative definite.

In this section we will examine some of the relationships between the algebraic stability of a method and its quadrature properties. Since the abscissae, $c_1, \cdots, c_s$, will always be assumed to be distinct, we will transform the stability matrix by the Vandermonde matrix V_s (whose (i, j) element is c_i^{j-1}) so that $R = V_s^T M V_s$. Consequently, under the assumption that $c_1, \cdots, c_s$ are distinct, a method is algebraically stable iff $b_1, \cdots, b_s \geqq 0$ and R is nonnegative. This congruence transformation simplifies the study of algebraic stability since there is a relationship between the order of a method and the number of zeros in the matrix R, expressed in the following result (which was given in Burrage [5]).

LEMMA 2. *If a Runge–Kutta method, with $c_1, \cdots, c_s$ distinct, is of order p, then the (l, m) element of R is zero for all l and m such that $l + m \leqq p$.*

We can now state

THEOREM 1. *If a Runge–Kutta method satisfying $B(2)$ and either $C(v)$ or $D(v)$ is algebraically stable, then $B(2v-1)$ must hold.*

Proof. Let r_{lm} be the (l, m) element of R; then

$$r_{lm} = \sum_{i,j=1}^{s} b_i c_i^{l-1} a_{ij} c_j^{m-1} + \sum_{i,j=1}^{s} b_i c_i^{m-1} a_{ij} c_j^{l-1} - \sum_{i=1}^{s} b_i c_i^{l-1} \sum_{i=1}^{s} b_i c_i^{m-1}, \tag{1}$$

so that under the assumption $C(v)$

$$r_{lm} = \frac{1 + g_{l+m} - (1 + g_l)(1 + g_m)}{lm} \quad \text{for } l \leqq v \text{ and } m \leqq v. \tag{2}$$

Furthermore, as $B(2)$ holds,

$$r_{11} = 2 \sum_{i=1}^{s} b_i c_i - \left(\sum_{i=1}^{s} b_i\right)^2 = 0,$$

so R being nonnegative implies $r_{l1} = 0$ for $l = 2, \cdots, s$. Therefore, $g_k = 0$ for $k \leqq v + 1$, and so $r_{lm} = 0$ for all l and m such that $l + m \leqq v + 1$. Repeating this process for $m = 2, \cdots, v - 1$ and using the nonnegativeness of R we find that

$$g_k = 0 \quad \text{for } k \leqq 2v - 1.$$

If on the other hand $D(v)$ holds, then

$$r_{lm}=\frac{-g_{l+m}-g_m g_l}{lm} \quad \text{for } l\leqq v \text{ and } m\leqq v \tag{3}$$

and the same argument is valid. □

The condition $B(2)$ is crucial in the statement of this result since it ensures that at least $r_{11}=0$, and this acts as a starting value for the iterative proof. The result fails if only $B(1)$ holds, as illustrated by the following example with $u>\frac{1}{2}$:

$$\begin{array}{c|cc} u(1-1/\sqrt{3}) & u/2 & u(\frac{1}{2}-1/\sqrt{3}) \\ u(1+1/\sqrt{3}) & u(\frac{1}{2}+1/\sqrt{3}) & u/2 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}.$$

This method is algebraically stable and satisfies B(1) and C(2) but not B(2).

THEOREM 2. (i) *If a Runge–Kutta method satisfying $B(2)$ and $C(v)$ is algebraically stable then $D(v-1)$ must hold.*

(ii) *If a Runge–Kutta method satisfying $B(2)$ and $D(v)$ is algebraically stable then $C(v-1)$ must hold.*

Proof. (i) Since, by Theorem 1, the initial assumptions imply $B(2v-1)$, we find from (2) that

$$r_{lm}=0 \quad \text{for } l\leqq v \text{ and } m\leqq v, \quad \text{where } l+m\leqq 2v-1,$$

which implies (because algebraic stability implies R is nonnegative)

$$r_{lm}=0 \quad \text{for } l=1,\cdots,s \text{ and } m=1,\cdots,v-1,$$

or, with $C(v)$ in (1) and $g_m=0$ for $m\leqq 2v-1$,

$$\sum_{i,j=1}^{s} b_i c_i^{m-1} a_{ij} c_j^{l-1}=\frac{1}{m}\left(\frac{1+g_l}{l}-\frac{1+g_{l+m}}{l+m}\right) \quad \text{for } l\leqq s \text{ and } m\leqq v-1. \tag{4}$$

But since the internal abscissae are assumed to be distinct, $D(v-1)$ is equivalent to (4), which is obtained by multiplying by c_j^{l-1} and summing on j in $D(v-1)$.

(ii) The proof of (ii) is similar to (i) but is based on (3) instead of (2) and will be omitted. □

COROLLARY 1. *If a Runge–Kutta method satisfying $B(2)$ and either $C(v)$ or $D(v)$ is algebraically stable, then it must be of order $2v-1$.*

Proof. The result is a consequence of Lemma 1 and Theorems 1 and 2. □

Since the maximum order of a singly-implicit method is $s+1$ (see [13], for example), we have as a consequence of Corollary 1 that there cannot exist algebraically stable singly-implicit methods (satisfying $C(s-1)$), with more than 4 stages. Furthermore, if there does exist a 4-stage singly-implicit method that is algebraically stable it must be of order 5, which by [4] is impossible since there are no 4-stage A-stable singly-implicit methods of order 5. Thus there do not exist algebraically stable singly-implicit methods (satisfying $C(s-1)$) with order greater than 4. We will construct these families of methods in § 3. However, to determine whether there exist algebraically stable singly-implicit methods of order greater than 4 the number of C-type simplifying assumptions must be reduced, and hence the following results will prove useful.

THEOREM 3. *If a Runge–Kutta method of order $p(\geqq 3)$ is algebraically stable with positive weights, then $C([(p-1)/2])$ must hold.*

Proof. See Hairer [10]. □

THEOREM 4. *If a Runge–Kutta method of order $p(\geqq 3)$ is algebraically stable with positive weights, then $C([(p-1)/2])$, $B(p)$ and $D([(p-1)/2])$ must hold.*

Proof. The proof is a consequence of Theorem 3 and an analysis similar to that used in the proof of Theorem 2. □

Remarks (i). Suppose that in the construction of algebraically stable methods one of the weights, b_I say, is zero; then necessarily $a_{jI}=0, j=1,\cdots,s, j\neq I$ (otherwise the stability matrix M is not nonnegative) and the ensuing method is degenerate (that is, it can be reduced to an $(s-1)$-stage method which produces exactly the same numerical results as an s-stage method). Thus in this paper we will assume that the methods being constructed are nondegenerate.

(ii) The above remark has important ramifications in the construction of algebraically stable nondegenerate DIRK's. In particular, since DIRK's cannot satisfy $C(2)$ (see [12], for example), we find from Theorem 3 that there do not exist algebraically stable DIRK's of order more than 4, as was first noted by Hairer [10]. The characterization of the family of algebraically stable DIRK's is given in § 4.

(iii) Theorem 4 implies that if there exist algebraically stable singly-implicit methods of order 5 or 6 they must satisfy $C(2)$ and $D(2)$. We will not attempt this construction, but note that Hairer and Wanner [11] have succeeded in constructing algebraically stable singly-implicit methods of orders 5 and 6. But the question of whether there exist algebraically stable singly-implicit methods of order 7 or more remains unsolved.

3. Algebraically stable singly-implicit methods. In this section we will construct s-stage algebraically stable singly-implicit methods of order s and $s+1$ for $s\leqq 3$ which satisfy $C(s-1)$. Since there cannot exist s-stage algebraically stable singly-implicit methods of order s satisfying $C(s-1)$ for $s>4$, the construction of higher order algebraically stable methods is difficult. But, as noted in Remark (iii) above, Hairer and Wanner have constructed 5-stage algebraically stable singly-implicit methods of orders 5 and 6 satisfying $C(2)$ and $D(2)$.

I. The method

$$\begin{array}{c|c} \lambda & \lambda \\ \hline & 1 \end{array} \tag{5}$$

is trivially singly-implicit and algebraically stable if and only if $\lambda \geqq \frac{1}{2}$. If $\lambda=\frac{1}{2}$ the method is of order 2.

II. The family of 2-stage singly-implicit methods of order 2 or more satisfying $C(1)$ is given by (see [4])

$$\begin{array}{c|c} \begin{matrix} c_1 \\ c_2 \end{matrix} & \begin{bmatrix} 1 & c_1 \\ 1 & c_2 \end{bmatrix} \begin{bmatrix} 0 & -\lambda^2 \\ 1 & 2\lambda \end{bmatrix} \begin{bmatrix} 1 & c_1 \\ 1 & c_2 \end{bmatrix}^{-1} \\ \hline & \dfrac{(2c_2-1)}{2(c_2-c_1)} \qquad \dfrac{1-2c_1}{2(c_2-c_1)} \end{array}. \tag{6}$$

From [5] we find that such methods are algebraically stable if and only if

$$\lambda \geqq \frac{1}{4}, \qquad c_1c_2-\frac{c_1+c_2}{2}+\lambda^2-\lambda+\frac{1}{2}=0.$$

Furthermore, if $\lambda=(3+\sqrt{3})/6$ and $c_1c_2-(c_1+c_2)/2+\frac{1}{3}=0$, then this family is algebraically stable and has order 3.

III. The family of 3-stage singly-implicit methods of order 3 satisfying $C(2)$ is given by (see [4])

$$\begin{array}{c|c} c_1 & \\ c_2 & \begin{bmatrix} 1 & c_1 & c_1^2 \\ 1 & c_2 & c_2^2 \\ 1 & c_3 & c_3^2 \end{bmatrix} \begin{bmatrix} 0 & 0 & 2\lambda^3 \\ 1 & 0 & -6\lambda^2 \\ 0 & \frac{1}{2} & 3\lambda \end{bmatrix} \begin{bmatrix} 1 & c_1 & c_1^2 \\ 1 & c_2 & c_2^2 \\ 1 & c_3 & c_3^2 \end{bmatrix}^{-1} \\ c_3 & \\ \hline & b_1 \qquad\qquad b_2 \qquad\qquad b_3 \end{array}, \tag{7}$$

where

$$b_1 = \frac{c_2c_3-(c_2+c_3)/2+\frac{1}{3}}{(c_1-c_2)(c_1-c_3)}, \quad b_2 = \frac{c_1c_3-(c_1+c_3)/2+\frac{1}{3}}{(c_2-c_1)(c_2-c_3)}, \quad b_3 = 1-b_1-b_2.$$

To investigate the algebraic stability properties of these methods we give a constructional proof.

Since the method is of order 3, $r_{11}=r_{12}=r_{21}=0$, so that $R \geqq 0$ if and only if

$$\begin{aligned} &r_{13}=0, \quad r_{22}>0, \quad r_{22}r_{33}-r_{32}^2 \geqq 0, \\ \text{or} \quad & \\ &r_{13}=r_{22}=r_{32}=0, \qquad r_{33} \geqq 0. \end{aligned} \tag{8}$$

But from (1) we find, after some tedious manipulation,

$$r_{13}=\frac{g_4}{4}+2\lambda^3-3\lambda^2+\lambda-\frac{1}{12}, \qquad r_{22}=\frac{g_4}{4},$$

$$r_{32}=\lambda^3-2\lambda^2+\frac{3\lambda}{4}-\frac{1}{15}+\frac{g_5}{10}+\frac{3\lambda g_4}{4},$$

$$r_{33}=\frac{4\lambda^3}{3}-3\lambda^2+\frac{6\lambda}{5}-\frac{1}{9}-3\lambda^2 g_4+\frac{6\lambda g_5}{5},$$

where

$$\frac{g_4}{4}=\int_0^1 \prod_{j=1}^3 (c_j-c)\,dc, \qquad \frac{g_5}{5}=\int_0^1 c \prod_{j=1}^3 (c_j-c)\,dc+(c_1+c_2+c_3)\frac{g_4}{4}.$$

Now $\lambda = (3+2\sqrt{3}\cos(\pi/18))/6$ (≈ 1.06858) is a zero of $2\lambda^3-3\lambda^2+\lambda-\frac{1}{12}$, and it can be easily shown that the second condition in (8) holds if and only if

$$g_4=0, \quad \lambda=\lambda_1, \quad \frac{g_5}{10}=-\lambda_1^3+2\lambda_1^2-\frac{3\lambda_1}{4}+\frac{1}{15}, \quad \lambda_1=\frac{3+2\sqrt{3}\cos(\pi/18)}{6}. \tag{9}$$

Some more calculations give that the first condition in (8) is equivalent to

$$\frac{g_4}{4}=-2\lambda^3+3\lambda^2-\lambda+\frac{1}{12}, \qquad 2\lambda^3-3\lambda^2+\lambda-\frac{1}{12}<0,$$

$$\left(\frac{g_5}{10}\right)^2+2\left(\frac{g_5}{10}\right)\left(6\lambda^4-8\lambda^3+\lambda^2+\frac{\lambda}{2}-\frac{1}{15}\right)$$
$$+84\lambda^8-264\lambda^7+\frac{956\lambda^6}{3}-198\lambda^5+\frac{1148\lambda^4}{15}-\frac{304\lambda^3}{15}+\frac{53\lambda^2}{15}-\frac{31\lambda}{90}+\frac{37}{2700} \leqq 0.$$

The discriminant, Δ, of the quadratic in $g_5/10$ is given by

$$\frac{\Delta}{4} = -48\lambda^8 + 168\lambda^7 - \frac{728\lambda^6}{3} + 188\lambda^5 - \frac{253\lambda^4}{3} + \frac{6\lambda^3}{3} - \frac{41\lambda^2}{12} + \frac{5\lambda}{18} - \frac{1}{108}$$
$$= (-2\lambda^3 + 3\lambda^2 - \lambda + \tfrac{1}{12})(\lambda - \tfrac{1}{3})(\lambda - \tfrac{1}{6})(24(\lambda - \tfrac{1}{2})^3 + 1),$$

and since $2\lambda^3 - 3\lambda^2 + \lambda - \frac{1}{12} < 0$, $\Delta \geqq 0$ if and only if $\lambda \in [\frac{1}{3}, \lambda_1)$. Thus the first condition of (8) holds if and only if

$$\text{(10)} \quad \begin{aligned} &\frac{g_4}{4} = -2\lambda^3 + 3\lambda^2 - \lambda + \frac{1}{12}, \qquad \lambda \in \left[\frac{1}{3}, \lambda_1\right), \\ &-\frac{\sqrt{\Delta}}{2} \leqq \frac{g_5}{10} + 6\lambda^4 - 8\lambda^3 + \lambda^2 + \frac{\lambda}{2} - \frac{1}{15} \leqq \frac{\sqrt{\Delta}}{2}. \end{aligned}$$

Note that if $\lambda = \lambda_1$ then $\Delta = 0$ and $\lambda_1^3 - 2\lambda_1^2 + 3\lambda_1/4 - \frac{1}{15} = 6\lambda_1^4 - 8\lambda_1^3 + \lambda_1^2 + \lambda_1/2 - \frac{1}{15}$, so that (9) and (10) can be replaced by

$$\text{(11)} \quad \begin{aligned} &\frac{g_4}{4} = -2\lambda^3 + 3\lambda^2 - \lambda + \frac{1}{12}, \qquad \lambda \in \left[\frac{1}{3}, \lambda_1\right], \\ &-\frac{\sqrt{\Delta}}{2} \leqq \frac{g_5}{10} + 6\lambda^4 - 8\lambda^3 + \lambda^2 + \frac{\lambda}{2} - \frac{1}{15} \leqq \frac{\sqrt{\Delta}}{2}. \end{aligned}$$

In order to study the condition that $b_1, b_2, b_3 \geqq 0$, we note that the matrix $\operatorname{diag}(b_1, b_2, b_3)$ is congruent (under the transformation matrix V_3) to

$$\begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} \\ \frac{1}{2} & \frac{1}{3} & (1+g_4)/4 \\ \frac{1}{3} & (1+g_4)/4 & (1+g_5)/5 \end{bmatrix},$$

which is nonnegative if and only if

$$\frac{g_5}{10} \geqq 6\left(\frac{g_4}{4}\right)^2 + \frac{g_4}{4} - \frac{1}{360},$$

that is,

$$\text{(12)} \qquad \frac{g_5}{10} \geqq 24\lambda^6 - 72\lambda^5 + 78\lambda^4 - 40\lambda^3 + 12\lambda^2 - 2\lambda + \frac{11}{90}.$$

But in order to satisfy (11) we already require that

$$\frac{g_5}{10} \geqq -6\lambda^4 + 8\lambda^3 - \lambda^2 - \frac{\lambda}{2} + \frac{1}{15} - \frac{\sqrt{\Delta}}{2},$$

so that if, for $\lambda \in [\frac{1}{3}, \lambda_1]$,

$$-6\lambda^4 + 8\lambda^3 - \lambda^2 - \frac{\lambda}{2} + \frac{1}{15} - \frac{\sqrt{\Delta}}{2} \geqq 24\lambda^6 - 72\lambda^5 + 78\lambda^4 - 40\lambda^3 + 12\lambda^2 - 2\lambda + \frac{11}{90},$$

there is no further restriction on λ. This last inequality is equivalent to

$$-2[abc]^{1/2} \geqq -(ab + c),$$

where

$$a = -2\lambda^3 + 3\lambda^2 - \lambda + \tfrac{1}{12}, \quad b = 24(\lambda - \tfrac{1}{2})^3 + 1, \quad c = (\lambda - \tfrac{1}{3})(\lambda - \tfrac{1}{6}),$$

and is always true for $\lambda \in [\frac{1}{3}, \lambda_1]$, since a, b and c are nonnegative. Therefore, the family of methods of order 3 given by (7) is algebraically stable if and only if

$$\begin{gathered} \frac{g_4}{4} = -2\lambda^3 + 3\lambda^2 - \lambda + \frac{1}{12}, \qquad \lambda \in \left[\frac{1}{3}, \frac{3+2\sqrt{3}\cos(\pi/18)}{6}\right), \\ -\frac{\sqrt{\Delta}}{2} \leqq \frac{g_5}{10} + 6\lambda^4 - 8\lambda^3 + \lambda^2 + \frac{\lambda}{2} - \frac{1}{15} \leqq \frac{\sqrt{\Delta}}{2}, \end{gathered} \tag{13}$$

where

$$\frac{g_4}{4} = \int_0^1 \prod_{j=1}^3 (c_j - c)\, dc, \qquad \frac{g_5}{5} = \int_0^1 c \prod_{j=1}^3 (c_j - c)\, dc + (c_1 + c_2 + c_3)\frac{g_4}{4},$$

$$\Delta = 4(-2\lambda^3 + 3\lambda^2 - \lambda + \tfrac{1}{12})(\lambda - \tfrac{1}{3})(\lambda - \tfrac{1}{6})(24(\lambda - \tfrac{1}{2})^3 + 1).$$

Furthermore, if

$$\lambda = \lambda_1 = \frac{3+2\sqrt{3}\cos(\pi/18)}{6}, \quad g_4 = 0, \quad \frac{g_5}{10} = -\lambda_1^3 + 2\lambda_1^2 - \frac{3\lambda_1}{4} + \frac{1}{15},$$

which, after some calculations, can be written as

$$\begin{gathered} \lambda = \lambda_1 = \frac{3+2\sqrt{3}\cos(\pi/18)}{6}, \qquad c_3 = \frac{c_1c_2/2 - (c_1+c_2)/3 + \frac{1}{4}}{c_1c_2 - (c_1+c_2)/2 + \frac{1}{3}}, \\ c_2 = \frac{\phi - (c_1 - \frac{1}{2})\psi \pm [(c_1 - \frac{1}{2})^2\psi^2 - \phi\psi/3 + \phi^2/3]^{1/2}}{2\phi}, \\ \phi = \frac{c_1^2 - c_1 + \frac{1}{6}}{12}, \qquad \psi = -2\lambda_1^3 + 4\lambda_1^2 - \frac{3\lambda_1}{2} + \frac{5}{36}, \end{gathered} \tag{14}$$

then the method is algebraically stable and order 4.

EXAMPLE 1. An interesting selection of c_1, c_2, c_3 that satisfies (13) is $c_1 = \lambda(2-\sqrt{2})$, $c_2 = \lambda(2+\sqrt{2})$, $c_3 = 1-\lambda$.

Thus, the family of singly-implicit methods of order 3 given by

$$\begin{array}{c|ccc} \lambda(2-\sqrt{2}) & \lambda(4-\sqrt{2})/4 & \lambda(4-3\sqrt{2})/4 & 0 \\ \lambda(2+\sqrt{2}) & \lambda(4+3\sqrt{2})/4 & \lambda(4+\sqrt{2})/4 & 0 \\ 1-\lambda & (-\lambda^2(11\sqrt{2}+8)+4\lambda(1+2\sqrt{2})-\sqrt{2})/8\lambda & (\lambda^2(11\sqrt{2}-8)+4\lambda(1-2\sqrt{2})+\sqrt{2})/8\lambda & \lambda \\ \hline & b_1 & b_2 & b_3 \end{array},$$

where

$$b_1 = \frac{6\lambda^2(2+\sqrt{2}) - 3\lambda(3+\sqrt{2}) + 1}{12\lambda(3\sqrt{2}-2) - \sqrt{2}},$$

$$b_2 = \frac{6\lambda^2(\sqrt{2}-2) + 3\lambda(3-\sqrt{2}) - 1}{12\lambda(3\sqrt{2}+2) - \sqrt{2}},$$

$$b_3 = \frac{6\lambda^2 - 6\lambda + 1}{3(7\lambda^2 - 6\lambda + 1)}$$

can be shown to be algebraically stable if and only if $\lambda \in [(3+\sqrt{3})/6, \lambda_1]$. This method is a useful one, since, as suggested in [4], it can be used as an error estimator with the embedded method

$$\begin{array}{c|cc} \lambda(2-\sqrt{2}) & \lambda(4-\sqrt{2})/4 & \lambda(4-3\sqrt{2})/4 \\ \lambda(2+\sqrt{2}) & \lambda(4+3\sqrt{2})/4 & \lambda(4+\sqrt{2})/4 \\ \hline & (4\lambda(1+\sqrt{2})-\sqrt{2})/8\lambda & (4\lambda(1-\sqrt{2})+\sqrt{2})/8\lambda \end{array},$$

used to compute the numerical solutions. However, as can be seen from II, the embedded method is algebraically stable if and only if $\lambda=(3+\sqrt{3})/6$, in which case it is of order 3 and no error estimate is possible. Thus in this example if $\lambda \in ((3+\sqrt{3})/6, \lambda_1]$ the error estimating method is algebraically stable but the embedded method is only A-stable.

4. Algebraically stable DIRK's. In §§ 2 and 3 we managed to construct algebraically stable singly-implicit methods of order up to 4, but were unable to obtain any general results about the existence of higher order algebraically stable methods (although, as already noted, Hairer and Wanner [11] have succeeded in constructing algebraically stable methods of orders 5 and 6). However from various studies of the A-stability properties of singly-implicit methods it seems unlikely that there exist algebraically stable singly-implicit methods of order greater than 8. On the other hand we know from § 2 that there do not exist algebraically stable DIRK's of order greater than 4. Hence in this section we will construct the complete family of s-stage algebraically stable DIRK's of order s ($s=2$, 3 and 4). In doing so we will assume that the abscissae are distinct and that the weights are strictly positive, since zero weights together with the nonnegativeness of the stability matrix imply that a method is degenerate and can be reduced to a smaller stage method.

I. The family of 2-stage algebraically stable DIRK's of order 2 or more is given by (6) with $c_1=\lambda$, namely

$$\begin{array}{c|cc} \lambda & \lambda & \\ 1-\lambda & 1-2\lambda & \lambda \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}, \qquad \lambda \geqq \tfrac{1}{4}, \quad \lambda \neq \tfrac{1}{2}, \tag{15}$$

and if $\lambda=(3+\sqrt{3})/6$ the method is algebraically stable and of order 3.

II. In constructing a family of 3-stage algebraically stable DIRK's we will analyze the matrix R. Consider the method

$$\begin{array}{c|ccc} \lambda & \lambda & & \\ d_2+\lambda & d_2 & \lambda & \\ d_3+\lambda & d_3-a_{32} & a_{32} & \lambda \\ \hline & b_1 & b_2 & b_3 \end{array}, \tag{16}$$

where d_2 and d_3 are distinct and nonzero. It will have order 3 if and only if

$$\begin{aligned} &b_1=1-b_2-b_3, && b_2d_2^2+b_3d_3^2=\tfrac{1}{3}-\lambda+\lambda^2, \\ &b_2d_2+b_3d_3=\tfrac{1}{2}-\lambda, && b_3a_{32}d_2=\tfrac{1}{6}-\lambda+\lambda^2, \end{aligned} \tag{17}$$

so that, by Lemma 2, R is nonnegative if and only if

$$r_{13}=0, \quad r_{22} \geqq 0, \quad r_{22}r_{33}-r_{32}^2 \geqq 0, \quad r_{33} \geqq 0.$$

From (1) and (17) we find

$$r_{13}=(d_3+2\lambda-1)(d_2(\lambda-\tfrac{1}{2})+\lambda^2-\lambda+\tfrac{1}{3}).$$

If $d_2(\frac{1}{2}-\lambda)=\lambda^2-\lambda+\frac{1}{3}$, (17) gives

$$b_1=\tfrac{1}{2},\quad b_2=\tfrac{1}{2},\quad b_3=0,\quad \lambda^2-\lambda+\tfrac{1}{6}=0,$$

and the method is degenerate and can be reduced to (15). Hence a necessary condition for (16) to be algebraically stable is

$$d_3=1-2\lambda.$$

Letting

$$u=d_2+\lambda-\frac{1}{2},\qquad p=\lambda^3-\frac{3\lambda^2}{2}+\frac{\lambda}{2}-\frac{1}{24},$$

we obtain from (1)

$$\begin{aligned}
r_{22}&=-2p,\\
r_{32}&=u(\lambda^2-\lambda+\tfrac{1}{6})(1-4\lambda)-2p,\\
r_{33}&=2[(\lambda^2-\lambda+\tfrac{1}{6})u(1-4\lambda-u\lambda)+(\lambda^2-\lambda+\tfrac{1}{6})((\lambda-\tfrac{1}{2})^3+\tfrac{1}{24})-p],
\end{aligned}$$

so that R is nonnegative if and only if

$$\begin{aligned}
&p\leqq 0,\\
&(\lambda^2-\lambda+\tfrac{1}{6})[12(\lambda-\tfrac{1}{2})^2(\lambda-\tfrac{1}{3})(\lambda-\tfrac{1}{6})u^2+4p((\lambda-\tfrac{1}{2})^3+\tfrac{1}{24})]\leqq 0, \qquad (18)\\
&(\lambda^2-\lambda+\tfrac{1}{6})u(1-4\lambda-u\lambda)+(\lambda^2-\lambda+\tfrac{1}{6})\left(p+\frac{\lambda-\frac{1}{6}}{4}\right)-p\geqq 0.
\end{aligned}$$

(The last inequality is needed only if $p=0$, in which case $R\geqq 0$ if and only if $p=0$, $u=0$, $(\lambda^2-\lambda+\frac{1}{6})(\lambda-\frac{1}{6})\geqq 0$, that is $d_2=\frac{1}{2}-\lambda$, $\lambda=(3+2\sqrt{3}\cos(\pi/18))/6$.)

Now we saw in § 3 that a Runge–Kutta method of order 3 with distinct abscissae has positive weights if and only if

$$\frac{g_5}{10}>6\left(\frac{g_4}{4}\right)^2+\frac{g_4}{4}-\frac{1}{360},$$

$$\left(\frac{g_4}{4}=\int_0^1\prod_{j=1}^3(c_j-c)\,dc,\quad \frac{g_5}{5}=\int_0^1 c\prod_{j=1}^3(c_j-c)\,dc+(c_1+c_2+c_3)\frac{g_4}{4}\right).$$

Since $c_1=\lambda$, $c_2=u+\frac{1}{2}$, $c_3=1-\lambda$, this condition is equivalent to

$$(\lambda^2-\lambda+\tfrac{1}{6})(1-(12(\lambda-\tfrac{1}{2})u)^2)>0.$$

Rewriting the second inequality in (18) as

$$\left(\lambda^2-\lambda+\frac{1}{6}\right)\frac{(\lambda-\frac{1}{6})(\lambda-\frac{1}{3})(1-(12(\lambda-\frac{1}{2})u)^2)-48(\lambda^2-\lambda+\frac{1}{6})^3}{12}\geqq 0,$$

we obtain the following complete class of nondegenerate algebraically stable DIRK's of order 3 with distinct abscissae:

$$\begin{array}{c|ccc}
\lambda & \lambda & & \\
u+\frac{1}{2} & u+\frac{1}{2}-\lambda & \lambda & \\
1-\lambda & 1-2\lambda-\alpha & \alpha & \lambda \\
\hline
 & b_1 & b_2 & b_3
\end{array}, \qquad (19)$$

where

$$b_1=\frac{u(1-2\lambda)+\frac{1}{6}}{(2\lambda-1)(2\lambda-1-2u)},\qquad b_2=\frac{\lambda^2-\lambda+\frac{1}{6}}{(\lambda-\frac{1}{2})^2-u^2},$$

$$b_3=\frac{u(2\lambda-1)+\frac{1}{6}}{(2\lambda-1)(2\lambda-1+2u)},\qquad \alpha=b_2\frac{\lambda-\frac{1}{2}-u}{b_3}$$

and where λ and u are such that

$$\lambda-\tfrac{1}{2}\neq 0,\quad \lambda^2-\lambda+\tfrac{1}{6}\neq 0,\quad u^2\neq(\lambda-\tfrac{1}{2})^2,\quad (12(\lambda-\tfrac{1}{2})u)^2\neq 1,$$

$$1-[12(\lambda-\tfrac{1}{2})u]^2\leqq\frac{48(\lambda^2-\lambda+\frac{1}{6})^3}{(\lambda-\frac{1}{3})(\lambda-\frac{1}{6})},\qquad \lambda\in\left(\frac{1}{3},\frac{3+\sqrt{3}}{6}\right), \tag{20}$$

$$1-[12(\lambda-\tfrac{1}{2})u]^2\geqq\frac{48(\lambda^2-\lambda+\frac{1}{6})^3}{(\lambda-\frac{1}{3})(\lambda-\frac{1}{6})},\qquad \lambda\in\left(\frac{3+\sqrt{3}}{6},\frac{3+2\sqrt{3}\cos(\pi/18)}{6}\right).$$

Furthermore, if $\lambda=(3+2\sqrt{3}\cos(\pi/18))/6$, then the method given by (19) with $u=0$ is algebraically stable and order 4.

III. The construction of a family of 4-stage algebraically stable DIRK's follows along lines similar to II. Consider the method

$$\begin{array}{c|cccc}
\lambda & \lambda & & & \\
d_2+\lambda & d_2 & \lambda & & \\
d_3+\lambda & d_3-a_{32} & a_{32} & \lambda & \\
d_4+\lambda & d_4-a_{42}-a_{43} & a_{42} & a_{43} & \lambda \\
\hline
 & b_1 & b_2 & b_3 & b_4
\end{array}, \tag{21}$$

where the d_i are distinct and nonzero. As in Nørsett [12], we define

$$h_1=1,\qquad h_5=\frac{1}{24}-\frac{\lambda}{2}+\frac{3\lambda^2}{2}-\lambda^3,$$

$$h_2=\tfrac{1}{2}-\lambda,\qquad h_6=\frac{1}{12}-\frac{2\lambda}{3}+\frac{3\lambda^2}{2}-\lambda^3,$$

$$h_3=\tfrac{1}{6}-\lambda+\lambda^2,\qquad h_7=\frac{1}{8}-\frac{5\lambda}{6}+\frac{3\lambda^2}{2}-\lambda^3,$$

$$h_4=\tfrac{1}{3}-\lambda+\lambda^2,\qquad h_8=\frac{1}{4}-\lambda+\frac{3\lambda^2}{2}-\lambda^3.$$

If we let $x_1=b_3a_{32}$, $x_2=b_4a_{42}$, $x_3=b_4a_{43}$, (21) will have order 4 if and only if

$$b_1+b_2+b_3+b_4=1,\qquad x_1d_2+x_2d_2+x_3d_3=h_3,$$

$$b_2d_2+b_3d_3+b_4d_4=h_2,\qquad x_1d_2d_3+x_2d_2d_4+x_3d_3d_4=h_7,$$

$$b_2d_2^2+b_3d_3^2+b_4d_4^2=h_4,\qquad x_1d_2^2+x_2d_2^2+x_3d_3^2=h_6,$$

$$b_2d_2^3+b_3d_3^3+b_4d_4^3=h_8,\qquad b_4d_2a_{43}a_{32}=h_5.$$

The solution to this set of equations is

$$(b_2,b_3,b_4)=(h_2,h_4,h_8)D^{-1},\qquad b_1=1-b_2-b_3-b_4,$$
$$(x_1,x_2,x_3)=(h_3,h_7,h_6)E^{-1},\qquad d_4=1-2\lambda, \tag{22}$$

where

$$D=\begin{bmatrix} d_2 & d_2^2 & d_2^3 \\ d_3 & d_3^2 & d_3^3 \\ d_4 & d_4^2 & d_4^3 \end{bmatrix} \quad\text{and}\quad E=\begin{bmatrix} d_2 & d_2d_3 & d_2^2 \\ d_2 & d_2d_4 & d_2^2 \\ d_3 & d_3d_4 & d_3^2 \end{bmatrix}.$$

Since the method given by (21) and (22) is of order 4, then by Lemma 2 a necessary condition that R be nonnegative is

$$r_{14}=r_{23}=r_{24}=0.$$

From (1) and (22) these conditions are equivalent to

$$\begin{aligned}(23)\qquad & h_2d_2d_3d_4-h_4(d_2d_3+d_2d_4+d_3d_4)+h_8(d_2+d_3+d_4)-h_3d_2d_3+h_6(d_2+d_3)\\ &\qquad =2\lambda^4-4\lambda^3+\frac{7\lambda^2}{2}-\frac{3\lambda}{2}+\frac{1}{4},\end{aligned}$$

$$(24)\qquad -h_3d_4(d_2+d_3)+h_7(d_2+d_3+d_4)+h_6d_4-2\lambda^4+4\lambda^3-\frac{7\lambda^2}{2}+\frac{4\lambda}{3}-\frac{1}{6}=0,$$

$$\begin{aligned}(25)\qquad & -h_3d_4((d_2+d_3)^2+d_3(d_4-d_2))+h_7(d_2^2+d_3^2+d_4^2+d_3d_4)+h_6d_4(d_3+d_2)\\ &\qquad -2\lambda(-h_3d_2d_3+h_6(d_2+d_3))+4\lambda^5-9\lambda^4+9\lambda^3-\frac{19\lambda^2}{4}+\frac{5\lambda}{4}-\frac{1}{8}=0.\end{aligned}$$

Equation (23) is always satisfied if $d_4=1-2\lambda$, in which case (24) becomes

$$\left(\lambda^3-\frac{3\lambda^2}{2}+\frac{\lambda}{2}-\frac{1}{24}\right)(d_2+d_3+2\lambda-1)=0.$$

Now it can easily be shown from (22) and (25) that if $\lambda^3-3\lambda^2/2+\lambda/2-\frac{1}{24}=0$, at least one of the weights must be zero and the ensuing method is degenerate. Hence we must have $d_2+d_3=1-2\lambda$, and substituting for d_2 in (25) we obtain a quadratic in d_3, namely

$$\begin{aligned}(2\lambda-1)\Big[d_3^2\Big(-\lambda^2+\frac{\lambda}{2}-\frac{1}{12}\Big)-d_3\Big(3\lambda^3-\frac{7\lambda^2}{2}+\frac{7\lambda}{6}-\frac{1}{8}\Big)&\\ +(1-2\lambda)\Big(\lambda^3-\frac{5\lambda^2}{4}+\frac{5\lambda}{12}-\frac{1}{24}\Big)\Big]&=0,\end{aligned}$$

whose roots are

$$\tfrac{1}{2}-\lambda,\qquad \frac{-2\lambda^3+5\lambda^2/2-5\lambda/6+\frac{1}{12}}{\lambda^2-\lambda/2+\frac{1}{12}},$$

(where we have assumed $\lambda-\frac{1}{2}\neq 0$, since we require $d_4\neq 0$). Since $d_2+d_3=1-2\lambda$ and $d_2\neq d_3$ we have

$$(26)\qquad d_2=-\frac{\lambda(\lambda-\frac{1}{3})}{(2\lambda^2-\lambda+\frac{1}{6})},\qquad d_3=1-2\lambda-d_2.$$

Therefore, the method of order 4 given by (21), (22) and (26), namely

$$
(27)\qquad
\begin{array}{c|cccc}
\lambda & \lambda & & & \\
\lambda(\lambda-\frac{1}{2})^2/u & \lambda(\frac{1}{3}-\lambda)/2u & \lambda & & \\
\frac{1}{2}-p/u & a_{31} & -8p(\lambda-\frac{1}{4})/(\lambda(\lambda-\frac{1}{3})) & \lambda & \\
1-\lambda & a_{41} & a_{42} & u/((4\lambda-1)(b_2-\frac{1}{2})) & \lambda \\
\hline
 & \frac{1}{2}-b_2 & b_2 & b_2 & \frac{1}{2}-b_2
\end{array}
$$

where

$$
(28)\qquad
\begin{aligned}
&u=\lambda^2-\frac{\lambda}{2}+\frac{1}{12},\quad p=\lambda^3-\frac{3\lambda^2}{2}+\frac{\lambda}{2}-\frac{1}{24},\quad b_2=\frac{u^2}{2\lambda(\lambda-\frac{1}{3})(\lambda-\frac{1}{4})},\\
&a_{31}=\frac{\frac{1}{2}-\lambda-p/u+8p(\lambda-\frac{1}{4})}{\lambda(\lambda-\frac{1}{3})},\qquad a_{42}=\frac{(\lambda^2-\lambda+\frac{1}{6})/2+p/d_2}{d_2(\frac{1}{2}-b_2)},\\
&a_{41}=1-2\lambda-a_{42}-\frac{u}{(4\lambda-1)(b_2-\frac{1}{2})},\\
&\lambda-\tfrac{1}{2}\neq 0,\qquad p\neq 0,
\end{aligned}
$$

will have a matrix R whose rank is less than or equal to 2. In particular R has the form

$$\left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & R^* \end{array}\right],$$

where 0 is the 2×2 matrix of zeros, and if V_4^{-1} is assumed to be partitioned into 2×2 matrices as

$$\left[\begin{array}{c|c} A_1 & A_3 \\ \hline A_2 & A_4 \end{array}\right],$$

then

$$M=\left[\begin{array}{c|c} A_2^TR^*A_2 & A_2^TR^*A_4 \\ \hline A_4^TR^*A_2 & A_2^TR^*A_4 \end{array}\right].$$

Hence $R\geqq 0$ if and only if the 2×2 upper left-hand matrix of M is nonnegative, and so the nondegenerate method given by (27) and (28) is algebraically stable if and only if

$$
(29)\qquad
\begin{bmatrix} (\frac{1}{2}-b_2)(2\lambda-\frac{1}{2}+b_2) & b_2(d_2-\frac{1}{2}+b_2) \\ b_2(d_2-\frac{1}{2}+b_2) & b_2(2\lambda-b_2) \end{bmatrix}\geqq 0,\qquad 0<b_2<\tfrac{1}{2}.
$$

Some calculations show that $0<b_2<\frac{1}{2}$ if and only if

$$\lambda\in\left(\frac{6+\sqrt{6}-\sqrt{30+12\sqrt{6}}}{12},\frac{6-\sqrt{6}-\sqrt{30-12\sqrt{6}}}{12}\right)\approx(0.06190,\,0.23010)$$

or

$$\lambda\in\left(\frac{6-\sqrt{6}+\sqrt{30-12\sqrt{6}}}{12},\frac{6+\sqrt{6}+\sqrt{30+12\sqrt{6}}}{12}\right)\approx(0.36075,\,1.34635),$$

where the four endpoints of these intervals are the zeros of $\lambda^4-2\lambda^3+\lambda^2-\lambda/6+\frac{1}{144}$. But we also require $2\lambda\geqq b_2$, which together with the conditions that $0<b_2<\frac{1}{2}$ gives the following range of values for λ (accurate to 5 decimal places)

$$(0.11387, 0.22934) \cup (0.36075, 1.34635). \tag{30}$$

Some further computations show that the determinant of the matrix in (29) is

$$\frac{2(\lambda^2-\lambda/2+\frac{1}{24})(-\lambda^5+17\lambda^4/8-4\lambda^3/3+17\lambda^2/48-\lambda/24+\frac{1}{576})b_2}{\lambda(\lambda-\frac{1}{3})(\lambda-\frac{1}{4})^2}, \tag{31}$$

and the values of λ satisfying (30) and the nonnegativeness of (31) are given by $\lambda \in [(3+\sqrt{3})/12, \lambda_2]$, where λ_2 (≈ 1.28058) is the largest zero of $\lambda^5 - 17\lambda^4/8 + 4\lambda^3/3 - 17\lambda^2/48 + \lambda/24 - \frac{1}{576}$. Finally, we note that

$$2\lambda - \tfrac{1}{2} + b_2 = 4\lambda(\lambda-\tfrac{1}{3})(\lambda-\tfrac{1}{4})^2 + \frac{(\lambda^2-\lambda/2+\frac{1}{12})^2}{2\lambda(\lambda-\frac{1}{3})(\lambda-\frac{1}{4})}$$

is positive for all $\lambda \in [(3+\sqrt{3})/12, \lambda_2]$, so that the complete family of nondegenerate, algebraically stable DIRK's of order 4 is given by (27) and (28) with $\lambda \in [(3+\sqrt{3})/12, \lambda_2]$.

The results of this section can now be summarized in Table 1. The first column represents the number of stages of the DIRK, the second column represents the range of values of λ for which the method is algebraically stable, while the third, fourth and fifth columns give the values of λ for which the method is degenerate; algebraically stable and of order $s+1$; or algebraically stable, L-stable, and of order s, respectively. (The last column of figures can be found in [4].)

TABLE 1

s	λ	Degeneracy	Algebraic stability and order $s+1$	L-stability and order s
1	$[\frac{1}{2}, \infty)$		$\frac{1}{2}$	1
2	$[\frac{1}{4}, \infty)$	$\frac{1}{2}$	$(3+\sqrt{3})/6$	$(2\pm\sqrt{2})/2$
3	$(\frac{1}{3}, (3+2\sqrt{3}\cos(\pi/18))/6]$	$\frac{1}{2}, (3+\sqrt{3})/6$	$(3+2\sqrt{3}\cos(\pi/18))/6$	0.43587
4	$[(3+\sqrt{3})/12, \lambda_2]$	$\frac{1}{2}, (3+2\sqrt{3}\cos(\pi/18))/6$	—	0.57282

(Note that $\lambda_2 \approx 1.28058$, the largest zero of $\lambda^5-17\lambda^4/8+4\lambda^3/3-17\lambda^2/48+\lambda/24-1/576$.)

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