SIAM J. NUMER. ANAL.
Vol. 31, No. 3, pp. 876–891, June 1994

015

ORDER RESULTS FOR MONO-IMPLICIT RUNGE–KUTTA METHODS*

K. BURRAGE†, F. H. CHIPMAN‡, AND P. H. MUIR§

Abstract. The mono-implicit Runge–Kutta methods are a subclass of the well-known implicit Runge–Kutta methods and have application in the efficient numerical solution of systems of initial and boundary value ordinary differential equations. Although the efficiency and stability properties of this class of methods have been studied in a number of papers, the specific question of determining the maximum order of an s-stage mono-implicit Runge–Kutta method has not been dealt with. In addition to the complete characterization of some subclasses of these methods having a number of stages $s \leq 5$, a main result of this paper is a proof that the order of an s-stage mono-implicit Runge–Kutta method is at most $s + 1$.

Key words. Runge–Kutta methods, ordinary differential equations

AMS subject classification. 65L05

1. Introduction. Implicit Runge–Kutta (IRK) methods were first presented in [4] for use in the numerical solution of initial value ordinary differential equations. Since that time there has been considerable attention devoted to these methods. The reader is referred to [5] for an extensive review of these methods.

An IRK method can be used to compute an approximation to the solution of the initial value problem

$$y'(t) = f(y(t)), \qquad y(t_i) = y_i,$$

where $y(t) \in R^n$ and $f : R^n \to R^n$. (For convenience we will consider only autonomous systems.) Using an IRK method, we obtain an approximation, y_{i+1}, to the true solution, $y(t)$, evaluated at the point $t_{i+1} = t_i + h_i$, of the form

$$y_{i+1} = y_i + h_i \sum_{r=1}^{s} b_r f(\hat{y}_r), \tag{1.1}$$

where

$$\hat{y}_r = y_i + h_i \sum_{j=1}^{s} a_{r,j} f(\hat{y}_j), \qquad r = 1, \ldots, s. \tag{1.2}$$

These methods are often given in the form of a tableau containing their coefficients, which, for the above method, would have the following form:

* Received by the editors November 5, 1990; accepted for publication (in revised form) May 26, 1993. This work was supported by the Natural Sciences and Engineering Research Council of Canada.

† Department of Mathematics, Center for Industrial and Applied Mathematics and Parallel Computing, University of Queensland, Brisbane 4072, Australia (kb@math.uq.oz.au).

‡ Acadia University, Wolfville, Nova Scotia, Canada, B0P 1X0 (chipman@acadiau.ca).

§ Saint Mary's University, Halifax, Nova Scotia, Canada, B3H 3C3 (muir@husky1.stmarys.ca).

$$\begin{array}{c|ccc} c_1 & a_{1,1} & \dots & a_{1,s} \\ \vdots & \vdots & \vdots & \vdots \\ c_s & a_{s,1} & \dots & a_{s,s} \\ \hline & b_1 & \dots & b_s \end{array},$$

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

Let $b = (b_1, b_2, \dots, b_s)^T$, A be the $s \times s$ matrix whose (i,j)th component is $a_{i,j}$, and e be the vector of 1's of length s. Then $c = (c_1, c_2, \dots, c_s)^T$ can be expressed as $c = Ae$, and the stability function of the IRK method is given by

$$R(h) = 1 + hb^T(I - hA)^{-1}e.$$

Note that in (1.2) above, each stage, $\hat{y}_r$, is defined implicitly in terms of itself and the other stages. Hence in order to obtain approximate values for the stages it is necessary to solve a system of $n \cdot s$, in general, nonlinear equations. This is often done using some form of modified Newton iteration, which makes the calculation of the stages a somewhat computationally expensive process.

A number of interesting subclasses of the IRK methods have recently been identified and investigated in the literature. These methods represent attempts to trade-off the higher accuracy of the IRK methods for methods which can be implemented more efficiently. Examples of such methods are singly-implicit Runge–Kutta methods [2], diagonally implicit Runge–Kutta methods [20], and mono-implicit Runge–Kutta methods [10].

In [18], an alternative representation of the IRK methods known as *parameterized* implicit Runge–Kutta (PIRK) methods was presented. These have the form

$$y_{i+1} = y_i + h_i \sum_{r=1}^{s} b_r f(\hat{y}_r), \tag{1.3}$$

where

$$\hat{y}_r = (1 - v_r)y_i + v_r y_{i+1} + h_i \sum_{j=1}^{s} x_{r,j} f(\hat{y}_j), \qquad r = 1, \dots, s. \tag{1.4}$$

They are usually represented by a modified tableau; the above method would have the tableau

$$\begin{array}{c|c|ccc} c_1 & v_1 & x_{1,1} & \dots & x_{1,s} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_s & v_s & x_{s,1} & \dots & x_{s,s} \\ \hline & & b_1 & \dots & b_s \end{array},$$

where $c_i = v_i + \sum_{j=1}^{s} x_{i,j}$. Substituting for y_{i+1} from (1.3) in (1.4), it is easily seen that the PIRK method given above is equivalent to the IRK method with coefficient tableau

$$
\begin{array}{c|cccc}
c_1 & x_{1,1}+v_1b_1 & x_{1,2}+v_1b_2 & \dots & x_{1,s}+v_1b_s \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
c_s & x_{s,1}+v_sb_1 & x_{s,2}+v_sb_2 & \dots & x_{s,s}+v_sb_s \\
\hline
 & b_1 & b_2 & \dots & b_s
\end{array} .
$$

Let $v = (v_1, v_2, \dots, v_s)^T$ and X be the $s \times s$ matrix whose (i,j)th component is $x_{i,j}$. Then $c = Xe + v$ and, from [18], the stability function, $R(h)$, of a PIRK satisfies

$$R(h) = \frac{P(h, e-v)}{P(h, -v)},$$

where

$$P(h, w) = 1 + hb^T(I - hX)^{-1}w, \qquad w \in R^s.$$

If we impose on the PIRK methods the restriction that the matrix X be strictly lower triangular then the resultant methods are known as mono-implicit Runge–Kutta (MIRK) methods.

MIRK methods have been discussed in the literature by a number of different authors for more than a decade. A subclass of these methods was first suggested for use in the solution of initial value ODE problems in [6]. The full MIRK class was presented for initial value problems in [1] (where they were called implicit endpoint quadrature formulas) and [10]. See [18] for a survey of these methods. It appears that, for initial value ODE problems, the computational costs associated with the use of MIRK methods are comparable to those of the best implementations of the more general IRK methods, such as described in [5]. MIRK methods have been considered for boundary value ODEs in [7]–[9], [11], [13], and [16]. For BVODEs, these methods can be implemented at a cost comparable to that of explicit Runge–Kutta methods (see [13]). MIRK methods have been used in the implementation of a software package, for the numerical solution of BVODEs, using deferred corrections, called HAGRON [7], [8], [12]. More recently, the MIRK methods have been used in a software package which employs continuous extensions of these methods (see [19]) to provide defect control for the numerical solution of BVODEs (see [14]).

Much of the above work has been concerned with the identification of particular MIRK methods and the investigation of their efficient implementation. As well, there has been some investigation of the forms of the order conditions for these methods, as they relate to the well-known Butcher conditions for the standard IRK methods, in [1] and [16]. However, a complete characterization of low-order MIRK methods has not been undertaken, as has been done for low-order explicit Runge–Kutta methods in [5]. This characterization is important because it allows an analysis of the resultant families to determine new methods representing potential improvements upon those currently available. Furthermore, the question of the maximum order of an s-stage MIRK has not been answered. In [17], it was conjectured that this maximum order is $s + 1$ and in [7] the maximum order question was identified as a significant open problem in the study of MIRK methods.

In §2 we present characterizations for several subclasses of MIRK methods having a small number of stages. In §3 we present some general results on the maximum order of an s-stage MIRK method, and show that an upper bound for the maximum order is $s+1$. In §4 we give some conclusions and suggestions for future work.

2. Low-order mono-implicit Runge–Kutta methods. In this section we present characterizations for a number of families of MIRK methods, having 1, 2, 3, 4, or 5 stages.

For the standard IRK method to have *at least* stage order p, it must satisfy the conditions $B(p)$ and $C(p)$ (see, e.g., [5, p. 289]), where

$$B(p) : b^T c^{k-1} = 1/k, \qquad k = 1, \dots, p,$$
$$C(p) : Ac^{k-1} = c^k/k, \qquad k = 1, \dots, p,$$

where $c^k = (c_1^k, c_2^k, \dots, c_s^k)$. For a MIRK method to have *at least* stage order p, it must satisfy the conditions, $B(p)$, as given above, and the following form of the $C(p)$ conditions,

$$C(p) : v + kXc^{k-1} = c^k, \qquad k = 1, \dots, p,$$

since for a MIRK method expressed in standard IRK form, we have $A = X + vb^T$. If, in addition, either of the conditions $B(p+1)$ or $C(p+1)$ do not hold, then either class of methods has *exactly* stage order p. Throughout this paper, unless explicitly stated otherwise, all references to order or stage order should be interpreted to be *exact* order or *exact* stage order. Also, for an IRK or MIRK method to be of classical order *at least* $p+1$, it is sufficient for the method to satisfy $B(p+1)$ and $C(p)$. See [5, pp. 214–219].

It has recently become clear (see, for example, [15]) that, in addition to the usual Runge–Kutta order concept, it is important to take into consideration the stage order of the Runge–Kutta method, at least in the context of solving stiff systems of differential equations. The basic idea is that a pth order Runge–Kutta method with stage order q, $(q < p)$ when applied to a stiff ODE system, can yield errors of order q or $q+1$, rather than the expected order p (see [15]). Thus, in searching for new methods it is important to require relatively high stage order. For a pth-order method, we would like to require stage order $p-1$ because the order reduction phenomenon is then not a concern and the order conditions needed to derive such a method are reduced to simply the quadrature conditions. Despite the advantages of having methods with high stage order, the following theorem shows that there is no point in searching for methods with stage order higher than 3.

THEOREM 2.1. (i) *A* MIRK *method having at least stage order* 2 *must have* $c_1 = 0$ *or* $c_1 = 1$; (ii) *a* MIRK *method having at least stage order* 3 *must have* $x_{2,1} = 0$ *and either* $c_1 = 0, c_2 = 1$ *or (equivalently)* $c_1 = 1, c_2 = 0$; *and* (iii) *the maximum stage order of an s-stage* MIRK *method is* $\min(s, 3)$.

Proof. (i) The stage order 2 conditions for a MIRK method are $v + Xe = c$, and $v + 2Xc = c^2$. The first equation from each of these gives $v_1 = c_1$ and $v_1 = c_1^2$ from which it follows that $c_1 = 0$ or 1.

(ii) The stage order 3 conditions are $v + Xe = c$, $v + 2Xc = c^2$, and $v + 3Xc^2 = c^3$. From (i) we have either $c_1 = 0$ or $c_1 = 1$. If $c_1 = 0$ then the second equation from each of these is $v_2 + x_{2,1} = c_2$, $v_2 = c_2^2$, and $v_2 = c_2^3$, from which it follows that $x_{2,1} = 0$, and $c_2 = 1$, so that the first and second stages are not the same. A similar argument holds for the case where $c_1 = 1$.

(iii) For $s = 1$ or 2, an s-stage MIRK method can only satisfy, simultaneously, at most, either $C(s+1)$ and $B(s)$, or $C(s)$ and $B(s+1)$. In either case this implies that the stage order is s. For $s \geq 3$, suppose the MIRK method has at least stage order 4. Then it must satisfy the $C(4)$ conditions which are $v + Xe = c$, $v + 2Xc = c^2$,

$v + 3Xc^2 = c^3$, and $v + 4Xc^3 = c^4$. Again from (i) we have either $c_1 = 0$ or $c_1 = 1$. For each value of c_1, it follows from (ii) that $x_{2,1} = 0$ and $c_2 = 1$ if $c_1 = 0$, or $c_2 = 0$ if $c_1 = 1$, so that the second stage is different from the first. Repeating this process for the third equation from each set of $C(4)$ conditions we come to the conclusion that the third stage must be the same as either the first or the second stage, thus implying that the MIRK method has only $s-1$ distinct stages, a contradiction. Hence the stage order of an s-stage MIRK method, with $s \geq 3$, is at most 3. □

In §3 of this paper we will show that the maximum order of an s-stage MIRK method is order $s+1$; hence in the following discussion, any s-stage MIRK method of at least order $s+1$ is of order exactly $s+1$.

2.1. MIRK methods with 1 stage. For the class of one-stage MIRK methods, a family of methods of at least order 1, including the explicit and implicit Euler methods, is obtained when $b_1 = 1, v_1 = c_1$ with c_1 left as a free parameter. If we choose $c_1 = \frac{1}{2}$, then we obtain the unique one-stage MIRK method of maximum order 2, namely the midpoint rule.

2.2. MIRK methods with 2 stages. Specific examples of order 2 MIRK methods are the trapezoidal rule ($x_{2,1} = 0$, $c_1 = v_1 = 0$, $c_2 = v_2 = 1$, $b_1 = b_2 = \frac{1}{2}$) and a one-parameter family of second-order two-stage MIRK methods given in [1] (method II). A more interesting question involves searching for third-order MIRK methods with 2 stages. An example of such a method is the two-point Gauss–Radau IRK method (Radau IIA), given in MIRK form in [1] (method III).

In order to search for third-order methods we must examine the corresponding order conditions for a two-stage MIRK method. It is a straightforward process to convert the standard Butcher conditions for IRK methods (see [5, p. 234]) to modified Butcher conditions that can be applied directly to methods expressed in terms of the MIRK tableau, i.e., with the inclusion of the extra parameters $v_1, v_2, \ldots, v_s$. For example, for third-order two-stage MIRK methods we have the following conditions: the quadrature conditions, denoted as $B(3)$,

$$b_1 + b_2 = 1, \quad b_1 c_1 + b_2 c_2 = \tfrac{1}{2}, \quad b_1 {c_1}^2 + b_2 {c_2}^2 = \tfrac{1}{3},$$

and the condition,

$$b_2 x_{2,1} c_1 + \tfrac{1}{2}(b_1 v_1 + b_2 v_2) = \tfrac{1}{6}.$$

Solving the above system, we get the following one-parameter family of two-stage third-order MIRK methods (letting c_1 be the parameter):

$$\begin{array}{c|c|cc}
c_1 & c_1 & 0 & 0 \\
\dfrac{3c_1 - 2}{3(2c_1 - 1)} & \dfrac{36c_1^3 - 54c_1^2 + 27c_1 - 4}{9(2c_1 - 1)^3} & -\dfrac{2(3c_1^2 - 3c_1 + 1)}{9(2c_1 - 1)^3} & 0 \\
\hline
 & & \dfrac{1}{4(3c_1^2 - 3c_1 + 1)} & \dfrac{3(4c_1^2 - 4c_1 + 1)}{4(3c_1^2 - 3c_1 + 1)}
\end{array}.$$

From an examination of the order conditions for order 4, it can easily be seen that it is impossible to choose the one free parameter, c_1, so that the above family can be of at least fourth order. Thus, for two-stage MIRK methods the maximum order is 3.

The linear stability function associated with this family of methods is

$$R(z) = \frac{6(1 - 2c_1) + 2(2 - 3c_1)z + (1 - c_1)z^2}{6(1 - 2c_1) - 2(1 - 3c_1)z - c_1 z^2},$$

and the method is A-stable if and only if $c_1 > \frac{1}{2}$. Also, note that if $c_1^2 - c_1 + \frac{1}{6} = 0$ then $B(4)$ holds. This is the MIRK analogue of the two-stage Gauss method of order 4.

The above family of methods has at least stage order 1. To find third order methods having stage order 2, we must impose the $C(2)$ conditions on the family of third-order methods above. We find that the only members that have stage order 2 are obtained by choosing $c_1 = 1$ or 0 in the $C(1)$ family which gives, respectively, method III (from [1]) mentioned above (which is A-stable) and its reflection [21] (which is not A-stable).

2.3. MIRK methods with 3 stages. We will first search for three-stage methods having at least at least order 3 and at least stage order 2. It is then necessary and sufficient to impose the $B(3)$ and $C(2)$ conditions. The latter condition implies either $c_1 = 0$ or $c_1 = 1$. We consider the $c_1 = 1$ case, noting that its reflection will yield the $c_1 = 0$ case. We get the following three-parameter family of methods where c_2, c_3, and v_3 are the parameters, with the restriction that 1, c_2, and c_3 are all different.

$$
\begin{array}{c|c|ccc}
1 & 1 & 0 & 0 & 0 \\
c_2 & c_2(2-c_2) & c_2(c_2-1) & 0 & 0 \\
c_3 & v_3 & \dfrac{c_3(c_3-2c_2)+v_3(2c_2-1)}{2(1-c_2)} & \dfrac{v_3+c_3(c_3-2)}{2(c_2-1)} & 0 \\
\hline
 & & \dfrac{6c_2c_3-3c_3-3c_2+2}{6(c_2-1)(c_3-1)} & \dfrac{3c_3-1}{6(c_2-1)(c_2-c_3)} & \dfrac{3c_2-1}{6(c_3-1)(c_3-c_2)}
\end{array}
$$

The linear stability function is

$$R(z) = \frac{6\alpha + 2(\alpha - \beta)z + \beta(c_2 - 1)z^2}{6\alpha - 2(2\alpha + \beta)z + (\alpha + \beta(c_2 + 1))z^2 - \beta c_2 z^3},$$

where

$$\alpha = (c_3 - 1)(c_3 - c_2), \quad \text{and} \quad \beta = \tfrac{1}{2}(v_3 + c_3(c_3 - 2))(3c_2 - 1).$$

The methods are A-stable if and only if $\beta/\alpha > 0$ and $(3c_2 - 1)\beta/\alpha < \frac{1}{2}$. If we were to require stage order 3, thus making $c_2 = x_{2,1} = 0$, $v_3 = c_3^2(3 - 2c_3)$, $x_{3,1} = c_3^2(c_3 - 1)$, and $x_{3,2} = c_3(c_3 - 1)^2$, the resulting method is A-stable if and only if $c_3 > 1$. The reflection of this method, with $c_1 = 0$, can only be A-stable if $c_2 = 1$, and hence $x_{2,1} = 0$.

If we now search for three-stage, order 4 MIRK methods with at least stage order 2, we get a one-parameter family of methods with either $c_1 = 0$ or $c_1 = 1$. Considering the case $c_1 = 1$, we have the following one-parameter family (where the parameter is c_2 is a real number, satisfying $c_2 \neq \frac{1}{4}, \frac{1}{3}$, or 1):

$$\begin{array}{c|c|ccc}
1 & 1 & 0 & 0 & 0 \\
c_2 & c_2(2-c_2) & c_2(c_2-1) & 0 & 0 \\
\dfrac{2c_2-1}{6c_2-2} & \dfrac{\delta}{\gamma} & \dfrac{(1-2c_2)(1-4c_2)\beta}{2(c_2-1)\gamma} & \dfrac{(4c_2-1)\alpha}{2(c_2-1)\gamma} & 0 \\
\hline
 & & \dfrac{6c_2^2-6c_2+1}{6(4c_2-1)(c_2-1)} & \dfrac{-1}{6(c_2-1)\alpha} & \dfrac{2(3c_2-1)^3}{3(4c_2-1)\alpha}
\end{array},$$

where

$$\delta = 180c_2^4 - 240c_2^3 + 121c_2^2 - 26c_2 + 2, \qquad \gamma = 4(3c_2-1)^4,$$
$$\beta = 1 - 10c_2 + 24c_2^2 - 18c_2^3, \quad \text{and} \quad \alpha = 6c_2^2 - 4c_2 + 1.$$

The linear stability function for this family of methods is given by

$$R(z) = \frac{P(z,c_2)}{Q(z,c_2)} = \frac{12(1-3c_2) + 6(1-2c_2)z + (1-c_2)z^2}{12(1-3c_2) - 6(1-4c_2)z + (1-7c_2)z^2 + c_2z^3},$$

and the methods are A-stable if and only if $c_2 > \frac{1}{3}$ or $c_2 = 0$. The choice of $c_2 = 0$ gives stage order 3.

The $c_1 = 0$ case gives the stability function,

$$R(z) = \frac{Q(-z, 1-c_2)}{P(-z, 1-c_2)},$$

and hence methods that are only A-stable for the one choice $c_2 = 1$, the stage order 3 case. It is easy to show that this stage order 3 method is the only such fourth-order, three-stage method. It is given in [1] (method IV) and is obtained by choosing $c_1 = v_1 = 0$, $c_2 = v_2 = 1$, $x_{2,1} = 0$, $c_3 = v_3 = \frac{1}{2}$, and $x_{3,1} = -x_{3,2} = \frac{1}{8}$.

2.4. MIRK methods with 4 stages. As might be expected, is not difficult to obtain four-stage MIRK methods of order at least 4. Two examples are given in [1] (methods V and VII), both of which have stage order 2. Below we give a three-parameter family of four-stage methods of at least order 4 having stage order 3. These are obtained by imposing the B(4) and C(3) conditions. The parameters are c_3, c_4, and v_4, with the restrictions that $c_3 \neq c_4$, $c_3 \neq 0, \frac{1}{2}, 1$, and $c_4 \neq 0, 1$.

$$\begin{array}{c|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
c_3 & c_3^2(3-2c_3) & c_3(c_3-1)^2 & c_3^2(c_3-1) & 0 & 0 \\
c_4 & v_4 & \dfrac{\alpha}{6c_3} & \dfrac{\gamma}{6(c_3-1)} & \dfrac{\psi}{6c_3(c_3-1)} & 0 \\
\hline
 & & \dfrac{\delta}{12c_3c_4} & \dfrac{\beta}{12(1-c_3)(1-c_4)} & \dfrac{2c_4-1}{12c_3(c_4-c_3)(1-c_3)} & \dfrac{1-2c_3}{12c_4(c_4-c_3)(1-c_4)}
\end{array},$$

where

$$\alpha = 6c_4c_3 + v_4 - 3c_3v_4 - 3c_3c_4^2 + 2c_4^3 - 3c_4^2, \qquad \gamma = 3c_3(c_4^2 - v_4) - 2(c_4^3 - v_4),$$
$$\delta = 1 - 2(c_3 + c_4) + 6c_3c_4, \qquad \beta = 3 - 4(c_3 + c_4) + 6c_3c_4,$$

and
$$\psi = c_4^2(2c_4 - 3) + v_4.$$

The linear stability function is
$$R(z) = \frac{p_0 + p_1 z + p_2 z^2 + p_3 z^3}{q_0 + q_1 z + q_2 z^2 + q_3 z^3},$$
where
$$p_0 = q_0 = 12c_4(c_4-1)(c_4-c_3), \qquad p_1 = 6c_4(c_4-1)(c_4-c_3)-(c_4^2(2c_4-3)+v_4)(2c_3-1),$$
$$q_1 = -6c_4(c_4-1)(c_4-c_3) - (c_4^2(2c_4-3)+v_4)(2c_3-1),$$
$$p_2 = c_4(c_4-1)(c_4-c_3) + \tfrac{1}{3}(c_4^2(2c_4-3)+v_4)(c_3-2)(2c_3-1),$$
$$q_2 = c_4(c_4-1)(c_4-c_3) + \tfrac{1}{3}(c_4^2(2c_4-3)+v_4)(c_3+1)(2c_3-1),$$
$$p_3 = \tfrac{1}{6}(c_4^2(2c_4-3)+v_4)(2c_3-1)(c_3-1), \qquad q_3 = -\tfrac{1}{6}(c_4^2(2c_4-3)+v_4)c_3(2c_3-1).$$
The family will be A-stable if and only if $c_3 > \frac{1}{2}$ and $\psi(2c_3-1)/6c_4(c_4-1)(c_4-c_3) > 0$.

It is also possible to generate four-stage, fifth-order MIRK methods. However, from Theorem 2.1 it is only worthwhile to search for four-stage, fifth-order MIRK methods having at most stage order 3. Below we present a four-stage, fifth-order family of at least stage order 2, which includes a four-stage, fifth-order family of stage order 3. The stage order 2 family has two parameters, c_2 and c_3.

$$\begin{array}{c|c|cccc}
1 & 1 & 0 & 0 & 0 & 0 \\
c_2 & c_2(2-c_2) & c_2(c_2-1) & 0 & 0 & 0 \\
c_3 & c_3(2-c_3) + 2x_{3,2}(c_2-1) & c_3(c_3-1) - x_{3,2}(2c_2-1) & x_{3,2} & 0 & 0 \\
\frac{\alpha}{5\beta} & \frac{\alpha}{5\beta} - x_{4,1} - x_{4,2} - x_{4,3} & x_{4,1} & x_{4,2} & x_{4,3} & 0 \\
\hline
 & & 1 - b_2 - b_3 - b_4 & \frac{\delta(c_3)}{\psi(c_2,c_3)} & \frac{\delta(c_2)}{\psi(c_3,c_2)} & \frac{125\beta^4}{12\gamma}
\end{array},$$

where
$$\alpha = 10c_2c_3 - 5(c_2+c_3) + 3, \qquad \beta = 6c_2c_3 - 2(c_2+c_3) + 1,$$
$$\gamma = (5\beta - \alpha)(5c_2\beta - \alpha)(5c_3\beta - \alpha),$$
$$\delta(c) = 10c^2 - 8c + 1, \quad \text{where} \quad c = c_2 \quad \text{or} \quad c_3,$$
$$\psi(c,d) = 12(1-c)(d-c)(5c\beta - \alpha), \quad \text{where} \quad c,d = c_2,c_3 \quad \text{or} \quad c_3,c_2,$$
$$x_{3,2} = \frac{(2c_2c_3 + c_2 + c_3 - 1)(1-c_3)(c_2-c_3)}{(3c_2-1)(c_2-1)\delta(c_2)},$$
$$x_{4,1} = \frac{\alpha}{5\beta}\left(\frac{\alpha}{5\beta} - 1\right) - x_{4,3}(2c_3-1) - x_{4,2}(2c_2-1), \qquad x_{4,3} = \frac{\gamma\delta(c_2)}{625\beta^5(c_3-1)(c_2-c_3)},$$
and
$$x_{4,2} = \frac{(5\beta-\alpha)(5c_2\beta-\alpha)(5c_3-2) - 125\beta^3 x_{4,3}(3c_3-1)(c_3-1)}{125\beta^3(3c_2-1)(c_2-1)}.$$
There are several restrictions on the values of the two parameters: $c_2 \neq c_3$, $c_2 \neq \frac{1}{3}$, 1, $c_3 \neq 1$, $\delta(c_2) \neq 0$, $\beta \neq 0$, $\gamma \neq 0$, $\psi(c_2,c_3) \neq 0$, and $\psi(c_3,c_2) \neq 0$.

The linear stability function for this family is given by

$$R(z) = \frac{w_0 + w_1 z + w_2 z^2 + w_3 z^3}{t_0 - t_1 z - t_2 z^2 - t_3 z^3 - t_4 z^4},$$

where

$$w_0 = t_0 = 60\beta(3c_2 - 1),$$

$$w_1 = 12(3c_2 - 1)\alpha, \quad w_2 = 3\beta(3c_2 - 1) + 6(\alpha - 2\beta)(2c_2 - 1), \quad w_3 = (\alpha - 2\beta)(c_2 - 1)$$

and

$$t_1 = 12(3c_2 - 1)(5\beta - \alpha), \qquad t_2 = 6(\alpha - 2\beta)(4c_2 - 1) - 9\beta(3c_2 - 1),$$

$$t_3 = \beta(3c_2 - 1) - (7c_2 - 1)(\alpha - 2\beta), \qquad t_4 = c_2(\alpha - 2\beta).$$

The methods are A-stable if and only if $0 < (2\beta - \alpha)(2c_2 + 1)/\beta(3c_2 - 1) < \frac{1}{2}$.

A one-parameter four-stage, fifth-order, stage order 3 family, contained within the above family, is obtained simply by choosing $c_2 = 0$. In this case, the methods are A-stable if and only if $c_3 > 1$.

2.5. MIRK methods with 5 stages. We focus, in this section, on five-stage methods of maximum order 6. An example of such a method is given in [1] (Method VIII), where the stage order has the maximum value of 3. This method is generalized to a five-stage, sixth-order, one-parameter family of methods having stage order 3 in [16, Table 2]. In this section we complete the generalization of these methods by presenting a two-parameter family of five-stage, sixth-order methods having stage order 3. The parameters are c_3 and c_4; by choosing $c_3 = (1-p)/2$ and $c_4 = (1+p)/2$ we get the one-parameter family (with parameter p) given in [16]. The restrictions on the parameters c_3 and c_4 are $c_3 \neq 0, 1$, $c_4 \neq 0, 1$, $\alpha \neq \beta \neq 0$, $\eta(c_3) \neq 0$, $\eta(c_4) \neq 0$, $\psi(c_3, c_4) \neq 0$, $\psi(c_4, c_3) \neq 0$, $\delta(c_3) \neq 0$, and $\gamma(c_4) \neq 0$. The two-parameter family is given below.

$$\begin{array}{c|c|ccccc}
1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
c_3 & c_3^2(3 - 2c_3) & c_3(c_3 - 1)^2 & c_3^2(c_3 - 1) & 0 & 0 & 0 \\
c_4 & c_4^2(3 - 2c_4) + 6x_{4,3}c_3(c_3 - 1) & x_{4,1} & x_{4,2} & \dfrac{(c_3 + c_4 - 1)\psi(c_4, c_3)}{2\delta(c_3)\gamma(c_3)} & 0 & 0 \\
\dfrac{\alpha}{\beta} & \dfrac{\alpha}{\beta} - x_{5,1} - x_{5,2} - x_{5,3} - x_{5,4} & x_{5,1} & x_{5,2} & x_{5,3} & x_{5,4} & 0 \\
\hline
 & & b_1 & b_2 & b_3 & b_4 & b_5
\end{array},$$

where

$$x_{4,1} = c_4(c_4 - 1)^2 - x_{4,3}(3c_3 - 1)(c_3 - 1), \qquad x_{4,2} = c_4^2(c_4 - 1) - x_{4,3}(3c_3 - 2)c_3,$$

$$x_{5,1} = c_5(c_5 - 1)^2 - x_{5,3}(3c_3 - 1)(c_3 - 1) - x_{5,4}(3c_4 - 1)(c_4 - 1),$$

$$x_{5,2} = c_5^2(c_5 - 1) - x_{5,3}(3c_3 - 2)c_3 - x_{5,4}(3c_4 - 2)c_4,$$

$$x_{5,3} = \frac{1}{60b_5\delta(c_3)} - x_{4,3}\frac{b_4}{b_5} - x_{5,4}\frac{\delta(c_4)}{\delta(c_3)}, \qquad x_{5,4} = \frac{\alpha(\beta - \alpha)\gamma(c_3)\eta(c_3)\eta(c_4)}{\psi(c_4, c_3)\beta^6},$$

$$b_1 = \frac{5c_3^2(10c_4^2 - 12c_4 + 3) - 5c_3(12c_4^2 - 15c_4 + 4) + (15c_4^2 - 20c_4 + 6)}{60(c_3 - 1)(c_4 - 1)(\beta - \alpha)},$$

$$b_2 = \frac{5c_3^2(10c_4^2 - 8c_4 + 1) - 5c_3(8c_4^2 - 7c_4 + 1) + \gamma(c_4)}{60c_3c_4\alpha},$$

$$b_3 = \frac{\gamma(c_4)}{60\psi(c_3, c_4)\eta(c_3)}, \qquad b_4 = \frac{\gamma(c_3)}{60\psi(c_4, c_3)\eta(c_4)}, \qquad b_5 = \frac{\beta^5}{60\alpha(\beta - \alpha)\eta(c_3)\eta(c_4)},$$

and where

$$\alpha = 5c_4c_3 - 3(c_3 + c_4) + 2, \qquad \beta = 10c_3c_4 - 5(c_3 + c_4) + 3,$$

$$\gamma(c) = 5c^2 - 5c + 1, \quad \delta(c) = c(c-1)(2c-1), \quad \eta(c) = c\beta - \alpha,$$

and

$$\psi(c, d) = c(c-1)(c-d).$$

The linear stability function is

$$R(z) = \frac{w_0 + w_1z + w_2z^2 + w_3z^3 + w_4z^4}{t_0 - t_1z - t_2z^2 - t_3z^3 - t_4z^4},$$

where

$$w_0 = t_0 = 120(2c_3 - 1)\beta, \quad w_1 = 120(2c_3 - 1)\alpha, \quad t_1 = 120(2c_3 - 1)(5c_3c_4 - 2(c_3 + c_4) + 1),$$

$$w_2 = 12(20{c_3}^2c_4 - 25c_3c_4 + 7c_4 - 15c_3^2 + 18c_3 - 5),$$
$$t_2 = -12(20c_3^2c_4 - 15c_3c_4 + 2c_4 - 5c_3^2 + 3c_3),$$

$$w_3 = 2(10c_3^2c_4 - 16c_3c_4 + 4c_4 - 11c_3^2 + 13c_3 - 3),$$
$$t_3 = 2(10{c_3}^2c_4 - 4c_3c_4 - 2c_4 + c_3^2 - 5c_3 + 3),$$

$$w_4 = c_3(1 - c_3 - c_4), \qquad t_4 = (c_3 - 1)(1 - c_3 - c_4).$$

The methods are A-stable if and only if $c_3 < \frac{1}{2}$ and $(1 - c_3 - c_4)/\beta > 0$.

3. The maximum order of an s-stage MIRK method. In this section, we will present a proof giving an upper bound on the order of an s-stage MIRK method, as given in (1.3) and (1.4), with coefficients represented by the vectors, $c = (c_1, c_2, \ldots, c_s)^T$, $v = (v_1, v_2, \ldots, v_s)^T$, $b = (b_1, b_2, \ldots, b_s)^T$, and the strictly lower triangular $s \times s$ matrix X, whose (i, j)th component is $x_{i,j}$. As before, e is the vector of 1's of length s. The proof is based on a subset of the Runge–Kutta order conditions, which we now present. (See [3, Thm. 7] for a related result.)

LEMMA 3.1. *For an s-stage* MIRK *method having at least order $s + 2$,*

$$\text{(CTCs)} \quad b^TX^{q-p}(c^{p+1} - c) = b^TX^{q-p+1}((p+1)c^p - e), \quad p = 1, \ldots, s, \quad q = p, \ldots, s.$$

(We refer to these conditions as the"cabbage tree" conditions (CTCs), since they are based on the order conditions associated with the set of trees, each consisting of a trunk of "i" edges surmounted by a bunch of "j" edges.)

Proof. Among the order conditions that any Runge–Kutta method of order at least $s + 2$ must satisfy are

$$b^TA^{q-p+1}c^p = p!/(q+2)! \quad \text{and} \quad b^TA^{q-p}c^{p+1} = (p+1)!/(q+2)!.$$

Let $t = c^{p+1} - (p+1)Ac^p$. Then

$$b^T A^{q-p} t = 0, \qquad p = 1, \dots, s, \quad q = p, \dots, s,$$

giving (for a MIRK method, where $A = X + vb^T$)

$$\begin{aligned} b^T A^{q-p} t &= b^T (X + vb^T) A^{q-p-1} t = b^T X A^{q-p-1} t = b^T X^2 A^{q-p-2} t = \cdots \\ &= b^T X^{q-p} t = 0. \end{aligned}$$

Since, for a MIRK method, $v = c - Xe$, we get

$$b^T X^{q-p} \left(c^{p+1} - (p+1) X \left(c^p - \frac{e}{p+1} \right) - c \right) = 0,$$

from which the result follows. □

We note that since X is strictly lower triangular, the vector $b^T X^i$, $i = 1, \dots, s-1$ has at least i zero elements, in the last i positions. We are interested in the (potentially) nonzero elements only, and so shall denote by $y_i = (y_{i,1} \dots, y_{i,i})^T$, the vector of length i consisting of the first i elements of $b^T X^{s-i}$, $i = 1, \dots, s-1$.

With

$$V_k = \begin{pmatrix} c_1^2 - c_1 & c_2^2 - c_2 & \dots & c_k^2 - c_k \\ c_1^3 - c_1 & c_2^3 - c_2 & \dots & c_k^3 - c_k \\ \vdots & \vdots & \ddots & \vdots \\ c_1^{k+1} - c_1 & c_2^{k+1} - c_2 & \dots & c_k^{k+1} - c_k \end{pmatrix},$$

a k by k matrix, and

$$V'_{k-1} = \begin{pmatrix} 2c_1 - 1 & 2c_2 - 1 & \dots & 2c_{k-1} - 1 \\ 3c_1^2 - 1 & 3c_2^2 - 1 & \dots & 3c_{k-1}^2 - 1 \\ \vdots & \vdots & \ddots & \vdots \\ (k+1)c_1^k - 1 & (k+1)c_2^k - 1 & \dots & (k+1)c_{k-1}^k - 1 \end{pmatrix},$$

a k by $k-1$ matrix, the CTCs may be grouped and rewritten as

$$V_1 y_1 = 0, \tag{1}$$

$$V_2 y_2 = V'_1 y_1, \tag{2}$$

$$V_3 y_3 = V'_2 y_2, \tag{3}$$

$$\vdots$$

$$V_{s-1} y_{s-1} = V'_{s-2} y_{s-2}, \tag{$s-1$}$$

and finally

$$V'_{s-1} y_{s-1} = -\frac{1}{2} \begin{pmatrix} \frac{1}{3} \\ \frac{2}{4} \\ \vdots \\ \frac{s}{s+2} \end{pmatrix}, \tag{s}$$

where we note that CTC(k) consists of k equations, $k = 1, \dots, s$. In the remainder of this proof, the right-hand sides of some of the CTCs will reduce to the zero vector.

When it arises in CTC(k), or in equations involving the vector y_k, $\underline{0}$ will denote the zero vector of length k.

In the proof of the main result that follows, we need the following lemma.

LEMMA 3.2. *Consider the matrix V_k and suppose $c_i \neq c_j$ for $i \neq j$, $i,j = 1,\dots,k$.*

(a) *If $c_i^2 \neq c_i$ for all $i = 1,\dots,k$, then V_k is nonsingular.*

(b) *If $c_p^2 = c_p$ for exactly one index $p \in \{1,\dots,k\}$, and if $\hat{V}_k$ represents V_k with column p replaced by its derivative with respect to c_p, then $\hat{V}_k$ is nonsingular.*

(c) *If there exist two distinct indices $p, l \in \{1,\dots,k\}$, with $c_p^2 = c_p$ and $c_l^2 = c_l$ and $\tilde{V}_k$ represents $\hat{V}_k$ with column l replaced by its derivative with respect to c_l, then $\tilde{V}_k$ is nonsingular.*

Proof. Part (a) follows immediately from the fact that

$$\det(V_k) = \left(\prod_{i=1}^{k}(c_i^2 - c_i)\right)\left(\prod_{j<i}(c_i - c_j)\right).$$

Parts (b) and (c) follow from the above expression for $\det(V_k)$ and the fact that

$$\det(\hat{V}_k) = \frac{\partial}{\partial c_p}\det(V_k) \quad \text{and} \quad \det(\tilde{V}_k) = \frac{\partial^2}{\partial c_p \partial c_l}\det(V_k). \qquad \square$$

We are now in a position to present and prove the main result of this section.

THEOREM 3.3. *The maximum order of an s-stage* MIRK *method cannot exceed $s+1$.*

Proof. If $s = 1$ or 2, then the result follows from §§2.1 and 2.2. Hence we assume $s \geq 3$. Suppose there is an s-stage MIRK method of order at least $s+2$. We consider the CTCs one at a time.

CTC(1) states that $(c_1^2 - c_1)y_{1,1} = 0$, and hence at least one of these two factors must vanish. Suppose $c_1^2 - c_1 = 0$. Then, in fact, $y_{1,1}$ must also be zero, for consider CTC (2), which becomes

$$\begin{pmatrix} c_2^2 - c_2 \\ c_2^3 - c_2 \end{pmatrix} y_{2,2} = \begin{pmatrix} -1 \\ -1 \end{pmatrix} y_{1,1} \quad \text{or} \quad \begin{pmatrix} 1 \\ 2 \end{pmatrix} y_{1,1}.$$

If $y_{1,1} \neq 0$, then $c_2 = 0$ or 1, both of which lead to contradictions in the above equations. Hence $y_{1,1} = y_1 = 0$. This result holds independently of whether or not $c_1^2 = c_1$, $c_2^2 = c_2$, or $c_1 = c_2$.

Note that if the c_i are distinct and all different from zero or one, Lemma 3.2 and the CTCs from (1) through $(s-1)$ give $y_i = \underline{0}$ for all $i = 1,\dots,s-1$. CTC(s) then obviously fails to hold. Thus we see that if there is to be any possibility for a method of at least order $s+2$ to exist, we must satisfy at least one of the conditions

$$c_i^2 = c_i, i \in \{1,\dots,s-1\} \quad \text{or} \quad c_i = c_j \text{ for } i \neq j, \quad i,j \in \{1,\dots,s-1\}.$$

We shall refer to these as singularities of type I ($c_i^2 = c_i$) and type II ($c_i = c_j, i \neq j$). (Note that a type I singularity implies that $c_i = 0$ or 1.)

Consider the first type II singularity that we encounter, involving $c_k = c_i$ for some $i \in \{1,\dots,k-1\}$. Because columns i and k in V_k are identical, we modify CTC(k) by replacing $y_{k,i}$ with $y_{k,i} + y_{k,k}$, replacing c_k with any real value different from all the abscissae, and replacing $y_{k,k}$ with zero. In fact, we carry out these modifications on all the remaining CTCs, replacing each $y_{j,i}$ with $y_{j,i} + y_{j,k}$, c_k with a real value different from the abscissae, and each $y_{j,k}$ with zero, for $j = k, k+1, \dots, s-1$.

We remove all further type II singularities in this manner, and are left with a modified set of CTCs for which, in the remainder of this proof, we will use the same notation. Hence, even although a repeated abscissa c_k has been replaced by an arbitrary distinct value, we will still denote this new value by c_k. Likewise, some of the components of the y_i's no longer denote their original values.

If there is no type I singularity, we see that all the $y_i, i = 1, \dots, s-1$, must vanish, leading to a contradiction in CTC(s). Hence we must have at least one type I singularity. In fact, there can be at most two such singularities (with abscissae equal to 0 and 1), since any additional type I singularities could be considered type II and removed as such.

We now continue our examination of the (modified) CTCs and assume that the first type I singularity involves c_k, $k \in \{1, \dots, s-1\}$. Then $c_k^2 = c_k$ and CTC(k) gives

$$\begin{pmatrix} c_1^2 - c_1 & \dots & c_{k-1}^2 - c_{k-1} \\ \vdots & & \dots \\ c_1^k - c_1 & \dots & c_{k-1}^k - c_{k-1} \end{pmatrix} \begin{pmatrix} y_{k,1} \\ \vdots \\ y_{k,k-1} \end{pmatrix} = \underline{0},$$

and since this coefficient matrix is nonsingular,

$$y_{k,1} = \dots = y_{k,k-1} = 0 \quad \text{and} \quad y_{k,k} \text{ is arbitrary.}$$

If $k = s-1$, then the first two equations of CTC(s) cannot be satisfied and we have a contradiction. Hence $k \in \{1, \dots, s-2\}$ and CTC($k+1$) now gives

$$\begin{pmatrix} c_1^2 - c_1 & \dots & c_{k-1}^2 - c_{k-1} & 2c_k - 1 & c_{k+1}^2 - c_{k+1} \\ \vdots & & \vdots & \vdots & \vdots \\ c_1^{k+2} - c_1 & \dots & c_{k-1}^{k+2} - c_{k-1} & (k+2)c_k^{k+1} - 1 & c_{k+1}^{k+2} - c_{k+1} \end{pmatrix} \begin{pmatrix} y_{k+1,1} \\ \vdots \\ y_{k+1,k-1} \\ -y_{k,k} \\ y_{k+1,k+1} \end{pmatrix} = \underline{0}.$$

Clearly $y_{k+1,k}$ is arbitrary and its place has been taken by $-y_{k,k}$. Suppose that there is exactly one type I singularity present. Then the above coefficient matrix is seen to be nonsingular by Lemma 3.2, and thus we have $y_{k,k} = 0$, $y_{k+1,k}$ arbitrary, and all the remaining components of y_{k+1} equal to zero. If $k = s-2$, CTC(s) once again leads to a contradiction, and hence $k \in \{1, \dots, s-3\}$.

If we next consider CTC($k+2$), we get a similar structure,

$$\begin{pmatrix} c_1^2 - c_1 & \dots & c_{k-1}^2 - c_{k-1} & 2c_k - 1 & c_{k+1}^2 - c_{k+1} & c_{k+2}^2 - c_{k+2} \\ \vdots & & \vdots & \vdots & \vdots & \vdots \\ c_1^{k+3} - c_1 & \dots & c_{k-1}^{k+3} - c_{k-1} & (k+3)c_k^{k+2} - 1 & c_{k+1}^{k+3} - c_{k+1} & c_{k+2}^{k+3} - c_{k+2} \end{pmatrix} \begin{pmatrix} y_{k+2,1} \\ \vdots \\ y_{k+2,k-1} \\ -y_{k+1,k} \\ y_{k+2,k+1} \\ y_{k+2,k+2} \end{pmatrix} = \underline{0}.$$

Again, Lemma 3.2 gives $y_{k+1,k} = 0$ and all components of y_{k+2} equal to zero except the kth one, $y_{k+2,k}$, which is arbitrary. This same effect continues for each subsequent CTC and corresponding y_i vector, leading to the observation that y_{s-1} has all zero components, except for the kth one, which is arbitrary. Then CTC(s) becomes,

$$\begin{pmatrix} 2c_k - 1 \\ \vdots \\ (s+1)c_k^s - 1 \end{pmatrix} y_{s-1,k} = -\frac{1}{2} \begin{pmatrix} \frac{1}{3} \\ \frac{2}{4} \\ \vdots \\ \frac{s}{s+2} \end{pmatrix},$$

where $c_k = 0$ or 1. Clearly the first two equations of the above condition lead to a contradiction. Hence, if there is any chance for an s stage MIRK method to be of at least order $s+2$, there must be two type I singularities.

The final possibility is that there is a second type I singularity, which we will suppose involves $c_l, l \in \{k+1, \ldots, s-1\}$. That is $c_l^2 = c_l$ with $c_l \neq c_k$. Then CTC(l) has the form

$$\begin{pmatrix} c_1^2 - c_1 & \cdots & c_{k-1}^2 - c_{k-1} & 2c_k - 1 & c_{k+1}^2 - c_{k+1} & \cdots & c_{l-1}^2 - c_{l-1} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ c_1^l - c_1 & \cdots & c_{k-1}^l - c_{k-1} & lc_k^{l-1} - 1 & c_{k+1}^l - c_{k+1} & \cdots & c_{l-1}^l - c_{l-1} \end{pmatrix} \begin{pmatrix} y_{l,1} \\ \vdots \\ y_{l,k-1} \\ -y_{l-1,k} \\ y_{l,k+1} \\ \vdots \\ y_{l,l-1} \end{pmatrix} = \underline{0},$$

with $y_{l,k}$ and $y_{l,l}$, arbitrary. The above matrix is nonsingular by Lemma 3.2 and thus $y_{l-1,k} = 0$, and all components of y_l are zero, except for the kth and lth, which are arbitrary. If $l = s-1$, CTC(s) yields a contradiction. Hence $l \in \{k+1, \ldots, s-2\}$ and CTC($l+1$) becomes

$$\begin{pmatrix} c_1^2 - c_1 & \cdots & c_{k-1}^2 - c_{k-1} & 2c_k - 1 & c_{k+1}^2 - c_{k+1} & \cdots & c_{l-1}^2 - c_{l-1} & 2c_l - 1 \\ \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots \\ c_1^{l+2} - c_1 & \cdots & c_{k-1}^{l+2} - c_{k-1} & (l+2)c_k^{l+1} - 1 & c_{k+1}^{l+2} - c_{k+1} & \cdots & c_{l-1}^{l+2} - c_{l-1} & (l+2)c_l^{l+1} - 1 \end{pmatrix}$$

$$\times \begin{pmatrix} y_{l+1,1} \\ \vdots \\ y_{l+1,k-1} \\ -y_{l,k} \\ y_{l+1,k+1} \\ \vdots \\ y_{l+1,l-1} \\ -y_{l,l} \end{pmatrix} = \underline{0},$$

with $y_{l+1,k}$ and $y_{l+1,l}$ arbitrary. The coefficient matrix above is nonsingular by Lemma 3.2 and thus we have $y_{l,k} = y_{l,l} = 0$, and all components of y_{l+1} equal to zero, except the kth and lth, which are arbitrary. Obviously this effect continues through the subsequent CTCs, and we reach the conclusion that y_{s-1} has all components equal to zero, except the kth and lth, which are arbitrary. CTC(s) becomes

$$\begin{pmatrix} 2c_k - 1 \\ \vdots \\ (s+1)c_k^s - 1 \end{pmatrix} y_{s-1,k} + \begin{pmatrix} 2c_l - 1 \\ \vdots \\ (s+1)c_l^s - 1 \end{pmatrix} y_{s-1,l} = -\frac{1}{2} \begin{pmatrix} \frac{1}{3} \\ \frac{2}{4} \\ \vdots \\ \frac{s}{s+2} \end{pmatrix},$$

with $c_k = 0$ and $c_l = 1$, or $c_k = 1$ and $c_l = 0$. The first three equations in this system are then impossible to satisfy. This completes the final possibility for the existence of an s-stage, order at least $s + 2$ MIRK method, and we conclude that no such method can exist. $\square$

4. Conclusions. In this paper we have extended the knowledge of the class of mono-implicit Runge–Kutta methods in several ways. We have completely characterized many of the lower stage, lower-order families of this class which have optimal stage order. This is significant, when solving stiff problems for example, because it is now known that in this case the stage order rather than the classical order is the appropriate measure of the accuracy of the method (see [15]). These characterizations will be useful in an analysis for determination of new methods for use in a boundary value ODE code using defect control, under development by one of the authors (see [14]).

A general result giving an upper bound of 3 for the stage order of an s-stage MIRK method is given. A main result of this paper shows that the order of an s-stage MIRK method is at most $s + 1$. In §2 we have presented methods having $s = 1, 2, 3, 4$, and 5, for which this bound is met. We conjecture that the bound cannot be met for $s \geq 6$.

Future work in this area could include a systematic investigation of the linear and nonlinear stability properties of the various families of MIRK methods identified in §2, as well as possible further attempts to completely characterize low stage MIRK methods having lower stage orders. Also, an investigation of the possibility of embedded families of MIRK methods of various orders would be very useful for error estimation purposes in software implementations for both in the initial value and boundary value problem areas. (Some embedded families of MIRK methods have been presented in [1] and [16].)

Acknowledgment. We would like to thank the referees for many helpful suggestions.

REFERENCES

[1] W. M. G. VAN BOKHOVEN, *Efficient higher order implicit one-step methods for integration of stiff differential equations*, BIT, 20 (1980), pp. 34–43.

[2] K. BURRAGE, *A special family of Runge–Kutta methods for solving stiff differential equations*, BIT, 18 (1978), pp. 22–41.

[3] ———, *Order properties of implicit multivalue methods for ordinary differential equations*, IMA J. Numer. Anal., 8 (1989), pp. 43–69.

[4] J. C. BUTCHER, *Implicit Runge–Kutta processes*, Math. Comp., 18 (1964), pp. 50–64.

[5] ———, *The Numerical Analysis of Ordinary Differential Equations*, John Wiley and Sons, Toronto, 1987.

[6] J. R. CASH, *A class of implicit Runge–Kutta methods for the numerical integration of stiff differential systems*, J. Assoc. Comput. Mach., 22 (1975), pp. 504–511.

[7] ———, *On the numerical integration of nonlinear two-point boundary value problems using iterated deferred corrections, Part* 1: *A survey and comparison of some one-step formulae*, Comput. Math. Appl., 12a (1986), pp. 1029–1048.

[8] ———, *On the numerical integration of nonlinear two-point boundary value problems using iterated deferred corrections, Part* 2: *The development and analysis of highly stable deferred correction formulae*, SIAM J. Numer. Anal., 25 (1988), pp. 862–882.

[9] J. R. CASH AND D. R. MOORE, *A high order method for the numerical solution of two-point boundary value problems*, BIT, 20 (1980), pp. 44–52.

[10] J. R. CASH AND A. SINGHAL, *Mono-implicit Runge–Kutta formulae for the numerical integra-*

tion of stiff differential systems, IMA J. Numer. Anal., 2 (1982), pp. 211–227.

[11] J. R. CASH AND A. SINGHAL, *High order methods for the numerical solution of two-point boundary value problems*, BIT, 22 (1982), pp. 184–199.

[12] J. R. CASH AND M. H. WRIGHT, *A deferred correction method for nonlinear two-point boundary value problems: implementation and numerical evaluation*, SIAM J. Sci. Statist. Comput., 12 (1991), pp. 971–989.

[13] W. H. ENRIGHT AND P. H. MUIR, *Efficient classes of Runge–Kutta methods for two-point boundary value problems*, Computing, 37 (1986), pp. 315–334.

[14] ———, *A Runge–Kutta type boundary value ODE solver with defect control*, Department of Computer Science, Tech. Rep. 267/93, University of Toronto, Toronto, 1993.

[15] R. FRANK, J. SCHNEID, AND C. W. UEBERHUBER, *Order results for implicit Runge–Kutta methods applied to stiff systems*, SIAM J. Numer. Anal., 23 (1985), pp. 515–534.

[16] S. GUPTA, *An adaptive boundary value Runge–Kutta solver for first order boundary value problems*, SIAM J. Numer. Anal., 22 (1985), pp. 114–126.

[17] P. H. MUIR, *Implicit Runge–Kutta methods for two-point boundary value problems*, Ph.D. Thesis, Department of Computer Science, Tech. Rep. 175/84, University of Toronto, Toronto, 1984.

[18] P. H. MUIR AND W. H. ENRIGHT, *Relationships among some classes of IRK methods and their stability functions*, BIT, 27 (1987), pp. 403–423.

[19] P. H. MUIR AND B. OWREN, *Order barriers and characterizations for continuous mono-implicit Runge–Kutta schemes*, Math. Comp., Vol. 61, No. 204, (1993), pp. 675–699.

[20] S. P. NØRSETT, *Semi-explicit Runge–Kutta methods*, Mathematics and Computation No.6/74, University of Trondheim, Trondheim, Norway, 1974.

[21] R. SCHERER AND H. TÜRKE, *Reflected and transposed methods*, BIT, 23 (1983), pp. 262–266.