JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

ELSEVIER Journal of Computational and Applied Mathematics 87 (1997) 147–167

On the generation of mono-implicit Runge–Kutta–Nyström methods by mono-implicit Runge–Kutta methods

H. De Meyer*, G. Vanden Berghe, T. Van Hecke, M. Van Daele

Vakgroep Toegepaste Wiskunde en Informatica, Universiteit-Gent, Krijgslaan 281 - S9, B9000 Gent, Belgium

Received 13 June 1997; received in revised form 8 September 1997

Abstract

Mono-implicit Runge–Kutta methods can be used to generate implicit Runge–Kutta–Nyström (IRKN) methods for the numerical solution of systems of second-order differential equations. The paper is concerned with the investigation of the conditions to be fulfilled by the mono-implicit Runge–Kutta (MIRK) method in order to generate a mono-implicit Runge–Kutta–Nyström method (MIRKN) that is P-stable. One of the main theoretical results is the property that MIRK methods (in standard form) cannot generate MIRKN methods (in standard form) of order greater than 4. Many examples of MIRKN methods generated by MIRK methods are presented.

Keywords: ODE; Runge–Kutta methods; Runge–Kutta–Nyström methods; Mono-implicit Runge–Kutta (Nyström) methods; P-stability

AMS classification: 65L06

1. Introduction

Implicit Runge–Kutta (IRK) methods for first-order ODEs $y' = f(t, y)$ have been studied extensively in the past. The reader is referred to [2] for an extensive review of these methods. The concept of MIRK methods has been introduced by van Bokhoven [21], where they were called implicit endpoint quadrature rules, and by Cash and Singhal [5]. Burrage et al. [1] give a complete characterization of some subsclasses of these methods having a number of stages $s \leqslant 5$. One of the main results of their paper is a proof that the order of an s-stage MIRK method is at most $s+1$. Special classes of MIRK methods, where the stages are evaluated in equidistant points with integer values $0, 1, \ldots, s-1$ have been studied by the present authors [22]; they have shown that MIRK methods belonging to this subclass are completely equivalent to the previously introduced extended one-step methods [20, 13, 6, 7]. In [10] it has been shown that a one-parameter family

* Corresponding author. E-mail: hans.demeyer@rug.ac.be.

PII S0377-0427(97)00183-0

of double-stride L-stable methods of fourth-order, obtained by the coupling of three linear multistep methods [8] can also be included within the framework of MIRK methods.

P-stable methods for second-order ODEs of the form $y''=f(t,y)$ are constructed either by considering so-called symmetric hybrid methods [3, 4, 9, 17–19] or by using IRKN methods [12]. In the two previous papers [23, 24] the present authors have studied a special class of four-stage fourth-order P-stable MIRKN methods, which are characterized by stages evaluated at abscissas having integer values in the range 0–3. In the present paper, MIRKN methods are generated from existing MIRK methods. We investigate the conditions to be fulfilled by the MIRK method in order to generate a P-stable MIRKN method. One of the main results is the property that MIRK methods (in standard form) cannot generate MIRKN methods (in standard form) of order greater than 4. In Section 2 some definitions and general theorems concerning MIRK and MIRKN methods are given. Section 3 presents the conditions to generate, from MIRK methods, P-stable MIRKN methods, while in Section 4 examples of MIRKN methods, generated from previously published MIRK methods, are given.

2. Definitions and theorems

An implicit Runge–Kutta method (IRK) for the solution of the initial value problem $y'=f(t,y)$, $y(t_0)=y_0$, is of the form

$$y_{n+1}=y_n+h\sum_{r=1}^{s}b_r f(t_n+c_r h, Y_r)$$

with

$$Y_r=y_n+h\sum_{j=1}^{s}a_{rj}f(t_n+c_j h, Y_j), \quad r=1,2,\ldots,s.$$

An IRK is completely characterized by means of its Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & b^{\mathrm{T}} \end{array}$$

or, equivalently, by the triplet (c,A,b), where $c,b\in\mathbb{R}^s$, $A\in\mathbb{R}^{s\times s}$ and s denotes the number of stages of the method.

The following representation of IRK methods, known as *parametrized* IRK (PIRK) methods was presented by Muir et al. [16]:

$$y_{n+1}=y_n+h\sum_{r=1}^{s}b_r f(t_n+c_r h, Y_r), \tag{2.1}$$

where for $r=1,2,\ldots,s$,

$$Y_r=(1-v_r)y_n+v_r y_{n+1}+h\sum_{j=1}^{s}x_{rj}f(t_n+c_j h, Y_j), \tag{2.2}$$

with $v \in \mathbb{R}^s$. Hence, a s-stage PIRK method is completely determined by the tableau

$$\begin{array}{c|c|cccc} c_1 & v_1 & x_{11} & x_{12} & \cdots & x_{1s} \\ c_2 & v_2 & x_{21} & x_{22} & \cdots & x_{2s} \\ c_3 & v_3 & x_{31} & x_{32} & \cdots & x_{3s} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \\ c_s & v_s & x_{s1} & x_{s2} & \cdots & x_{ss} \\ \hline & & b_1 & b_2 & \cdots & b_s \end{array} \tag{2.3}$$

Comparing this representation with the description of a general IRK method by means of its Butcher tableau (c, A, b), it is easy to verify that for PIRK methods the relationship $A = X + vb^{\mathrm{T}}$ holds, i.e., $a_{ij} = x_{ij} + v_i b_j$. By requiring that X be a strictly lower triangular matrix, one obtains mono-implicit Runge–Kutta methods in what we will call *standard form* (SMIRK methods). More generally, an IRK method expressed in the form of a PIRK method is said to be mono-implicit if X is strictly lower triangular after a possible rearrangment of the rows and columns of X and a corresponding rearrangement of the elements of c, v and b.

Definition 1. (i) An IRK method with tableau (c, A, b) is mono-implicit in standard form (SMIRK) if there exists a strictly lower triangular matrix $X \in \mathbb{R}^{s \times s}$ and a vector $v \in \mathbb{R}^s$ such that A can be decomposed as

$$A = X + v\, b^{\mathrm{T}}. \tag{2.4}$$

(ii) An IRK method with tableau (c, A, b) is mono-implicit (MIRK) if there exists a permutation matrix $P \in \{0, 1\}^{s \times s}$ $(PP^{\mathrm{T}} = P^{\mathrm{T}}P = I)$ such that the IRK method with Butcher tableau $(Pc, PAP^{\mathrm{T}}, Pb)$ is in standard form, i.e., there exists a strictly lower triangular matrix X and a vector v such that

$$PAP^{\mathrm{T}} = X + vb^{\mathrm{T}}P^{\mathrm{T}}, \tag{2.5}$$

or, equivalently,

$$A = P^{\mathrm{T}}XP + P^{\mathrm{T}}v\, b^{\mathrm{T}}.$$

Thus, a MIRK method can be converted to an equivalent SMIRK by a permutation of the rows and columns of X and corresponding permutations of the elements of c, v and b. This corresponds to a relabelling of the stages of the MIRK method.

The general form of a s-stage implicit Runge–Kutta–Nyström (IRKN) method for the solution of the initial value problem $y'' = f(t, y)$, $y(t_0) = y_0$, $y'(t_0) = y_0'$, is

$$\begin{aligned} y_{k+1} &= y_k + h\, y_k' + h^2 \sum_{i=1}^{s} (\bar{b}_N)_i\, f(t_k + (c_N)_i\, h, Y_i), \\ y_{k+1}' &= y_k' + h \sum_{i=1}^{s} (b_N)_i\, f(t_k + (c_N)_i\, h, Y_i), \end{aligned} \tag{2.6}$$

whereby

$$Y_i = y_k + (c_N)_i\, h\, y'_k + h^2 \sum_{j=1}^{s} (a_N)_{ij}\, f(t_k + (c_N)_j h, Y_j), \quad i = 1, 2 \dots, s. \tag{2.7}$$

They can be represented in a compact way by their associated Butcher tableau

$$\begin{array}{c|c} c_N & A_N \\ \hline & \bar{b}_N^{\mathrm{T}} \\ & b_N^{\mathrm{T}} \end{array}$$

which will also be represented by the quadruplet $(c_N, A_N, \bar{b}_N, b_N)$. In order to distinguish the notation for MIRK and MIRKN methods, we have added a subscript N to the symbols occurring in the Butcher tableaus of MIRKN methods.

An IRKN method can also be written in parametrized form, namely [24],

$$\begin{aligned} Y_i = {} & [1 - (v_N)_i]\, y_k + (v_N)_i\, y_{k+1} + [(c_N)_i - (v_N)_i - (w_N)_i]\, h\, y'_k + (w_N)_i\, h\, y'_{k+1} \\ & + h^2 \sum_{j=1}^{s} (x_N)_{ij}\, f(t_k + (c_N)_j h, Y_j), \end{aligned} \tag{2.8}$$

and is also characterized by the tableau

$$\begin{array}{c|c|c|c} c_N & v_N & w_N & X_N \\ \hline & & & \bar{b}_N^{\mathrm{T}} \\ & & & b_N^{\mathrm{T}} \end{array}$$

where v_N and w_N are vectors with components $(v_N)_i$ and $(w_N)_i$, respectively, and where X_N is a matrix with elements $(x_N)_{ij}$. The relation between the two forms is $A_N = X_N + v_N \bar{b}_N^{\mathrm{T}} + w_N b_N^{\mathrm{T}}$. If X_N is strictly lower triangular then one obtains a system of equations that is implicit in the variables y_{n+1} and y'_{n+1}. If in addition $v_N \equiv 0$ or $w_N \equiv 0$, then we will call the resultant methods with tableau $(c_N, A_N, \bar{b}_N, b_N)$ standard mono-implicit RKN (SMIRKN) methods.

Definition 2. (i) An IRKN method with tableau $(c_N, A_N, \bar{b}_N, b_N)$ is mono-implicit in standard form (SMIRKN) if there exists a strictly lower triangular matrix $X_N \in \mathbb{R}^{s \times s}$ and either a vector $v_N \in \mathbb{R}^s$ such that A_N can be written as

$$A_N = X_N + v_N\, \bar{b}_N^{\mathrm{T}}, \tag{2.9}$$

or a vector $w_N \in \mathbb{R}^s$ such that A_N can be written as

$$A_N = X_N + w_N\, b_N^{\mathrm{T}}. \tag{2.10}$$

(ii) An IRKN method with tableau $(c_N, A_N, \bar{b}_N, b_N)$ is mono-implicit (MIRKN) if there exists a permutation matrix $P \in \{0,1\}^{s \times s}$ such that the IRKN method with Butcher tableau $(Pc_N, PA_N P^{\mathrm{T}}, P\bar{b}_N,$

Pb_N) is a SMIRKN method, i.e. there exists X_N, v_N such that

$$PA_NP^T = X_N + v_N \bar{b}_N^T P^T, \tag{2.11}$$

or there exists X_N, w_N such that

$$PA_NP^T = X_N + w_N b_N^T P^T. \tag{2.12}$$

Thus, a MIRKN method can be converted to an equivalent SMIRKN method through a relabelling of its stages.

Since a system of second-order differential equations of the type $y'' = f(x, y, y')$ is equivalent with the first-order system $y' = z$ and $z' = f(x, y, z)$, it is clear that any IRK method applied to the latter system can be seen as an IRKN method for the one-step integration of the former system. We say that such an IRKN method is generated by an IRK method. However, not all IRKN methods are generated by IRK methods [12]. The Butcher tableau of an IRKN method generated by an IRK method is itself completely determined by the Butcher tableau of the IRK method. Indeed, (see, e.g., [12, p. 260]):

Theorem 3. *If (c, A, b) with $c, b \in \mathbb{R}^s, A \in \mathbb{R}^{s\times s}$ is the Butcher tableau of a s-stage IRK method, then $(c_N, A_N, \bar{b}_N, b_N)$ with*

$$c_N = c, \quad b_N = b, \quad A_N = A^2, \quad \bar{b}_N^T = b^T A, \tag{2.13}$$

is the Butcher tableau of a s-stage IRKN method.

From here onward, we only consider IRKN methods which are generated by IRK methods. Obviously, the order of such an IRKN method is the same as the order of the underlying IRK method. The same property holds for the stage order, as may be seen from the following definition [12] and Theorem 3.

Definition 4. An IRK method has stage order $q \geqslant 1$ if it is of order at least q and if the conditions

$$Ac^k = \frac{1}{k+1} c^{k+1}, \quad k = 0, 1, \ldots, q-1,$$

are satisfied, whereby c^k denotes the (column) vector with entries c_i^k $(i = 1, 2, \ldots, s)$ and $e = c^0$ denotes the vector with unit entries.

An IRKN method has stage order $q \geqslant 2$ if it is of order at least q and if the conditions

$$A_N c_N^k = \frac{1}{(k+1)(k+2)} c_N^{k+2}, \quad k = 0, 1, \ldots, q-2,$$

are satisfied.

In contrast with order and stage order, the property of mono-implicitness is not automatically preserved in the process of constructing IRKN methods from IRK methods. Therefore, we want to investigate the conditions under which a SMIRK method can generate a SMIRKN method of type

(2.9) or (2.10). We want to consider also the more general problem of generating a MIRKN method of type (2.11) or (2.12) by a SMIRK method, or equivalently, generating a SMIRKN method of type (2.9) or type (2.10) by a MIRK method. This equivalence is made explicit by the following theorem:

Theorem 5. *Suppose the SMIRK method characterized by* (c,A,b) *generates a MIRKN method characterized by* $(c_N,A_N,\bar{b}_N,b_N)$, *with permutation matrix* P, *strictly lower triangular matrix* X_N, *and vector* v_N *or* w_N *such that* $PA_NP^{\mathrm{T}}=X_N+v_N\bar{b}_N{}^{\mathrm{T}}P^{\mathrm{T}}$ *or* $PA_NP^{\mathrm{T}}=X_N+w_Nb_N^{\mathrm{T}}P^{\mathrm{T}}$. *Then the method characterized by* (Pc,PAP^{T},Pb) *is a MIRK method (with permutation matrix* $Q=P^{\mathrm{T}}$*) that generates a SMIRKN method characterized by* $(c_N',A_N',\bar{b}_N',b_N')$ *with strictly lower triangular matrix* X_N, *and vector* v_N *or* w_N, *such that* $A_N'=X_N+v_N\bar{b}_N'^{\mathrm{T}}$ *or* $A_N'=X_N+w_Nb_N'^{\mathrm{T}}$.

Proof. We first prove the theorem for the case of a MIRKN method of type (2.11). Since (c,A,b) characterizes a SMIRK method, there exist a X and v such that $A=X+v\,b^{\mathrm{T}}$. The generated MIRKN method with $(c_N,A_N,\bar{b}_N,b)$ satisfies for a certain P, X_N (strictly lower triangular), and v_N condition (2.11), which due to (2.13) can be written as

$$PA^2P^{\mathrm{T}}=X_N+v_N\,\bar{b}_N^{\mathrm{T}}P^{\mathrm{T}}=X_N+v_N\,b^{\mathrm{T}}AP^{\mathrm{T}}. \tag{2.14}$$

Substituting for A in terms of X, v and b, and rearranging, one finds

$$X_N=P[X+(v-P^{\mathrm{T}}v_N)\,b^{\mathrm{T}}][X+v\,b^{\mathrm{T}}]P^{\mathrm{T}}. \tag{2.15}$$

We now consider the IRK method associated with the triplet (c',A',b') with

$$c'=Pc,\quad A'=PAP^{\mathrm{T}},\quad b'=Pb,$$

and whereby P is the same permutation matrix as before. This method is a MIRK method since, one has

$$P^{\mathrm{T}}A'P=A=X+v\,b^{\mathrm{T}}=X+vb'^{\mathrm{T}}P,$$

which is of the form (2.5) with permutation matrix P^{T}. This MIRK method generates an IRKN method with quadruplet $(c_N',A_N',\bar{b}_N',b_N')$ whereby

$$c_N'=c',\quad A_N'=A'^2,\quad \bar{b}_N'^{\mathrm{T}}=b'^{\mathrm{T}}A',\quad b_N'=b'.$$

With the help of (2.14), it follows that

$$A_N'=(PAP^{\mathrm{T}})^2=PA^2P^{\mathrm{T}}=X_N+v_N\,\bar{b}_N^{\mathrm{T}}P^{\mathrm{T}}.$$

Since

$$\bar{b}_N'^{\mathrm{T}}=b'^{\mathrm{T}}A'=b^{\mathrm{T}}P^{\mathrm{T}}PAP^{\mathrm{T}}=b^{\mathrm{T}}AP^{\mathrm{T}}=\bar{b}_N^{\mathrm{T}}P^{\mathrm{T}},$$

one finally obtains

$$A_N'=X_N+v_N\,\bar{b}_N'^{\mathrm{T}},$$

which proves that $(c_N',A_N',\bar{b}_N',b_N')$ characterizes a SMIRKN method with the same X_N and v_N as before.

The proof for the case of a MIRKN method of type (2.12) goes in a completely analogous way. Instead of (2.14), however, the MIRKN should now be written as

$$PA^2P^{\mathrm{T}} = X_N + w_N\, b_N^{\mathrm{T}} P^{\mathrm{T}}, \tag{2.16}$$

and substituting on both sides the expression of A in terms of X and v, one obtains

$$X_N = P[X + v\,b^{\mathrm{T}}][X + v\,b^{\mathrm{T}}]P^{\mathrm{T}} - w_N\, b^{\mathrm{T}} P^{\mathrm{T}}. \tag{2.17}$$

The end of the proof proceeds analogously. □

Expressions (2.15) and (2.17) will be useful for proving certain existence conditions. From Theorem 5 it also follows that one should not be concerned with the generation of nonstandard MIRKN methods by nonstandard MIRK methods, since by means of a suitable permutation, it is always possible to bring either the MIRK method or the MIRKN method into a standard form. In the following sections, we will investigate the particular case of SMIRKN methods generated by SMIRK methods.

In [1] it is shown that the stage order of a SMIRK method is at most 3. More precisely, the following theorem is given there:

Theorem 6. (i) *A SMIRK method having at least stage order* 2 *must have* $c_1 = 0$ *or* $c_1 = 1$;
(ii) *A SMIRK method having at least stage order* 3 *must have* $x_{21} = 0$ *and either* $c_1 = 0, c_2 = 1$ *or (equivalently)* $c_1 = 1, c_2 = 0$;
(iii) *the maximum stage order of a s-stage MIRK method is min*$(s, 3)$.

Since the stage order is preserved in the generation of MIRKN methods by MIRK methods, certain statements of Theorem 6 related to MIRK methods can be straightforwardly transferred to the MIRKN methods generated by them.

Theorem 7. (i) *A MIRKN method generated by a SMIRK method having at least stage order* 2, *has at least stage order* 2 *and must have* $(c_N)_1 = 0$ *or* $(c_N)_1 = 1$;
(ii) *a MIRKN method generated by a SMIRK method having at least stage order* 3, *has at least stage order* 3 *and must have either* $(c_N)_1 = 0, (c_N)_2 = 1$ *or (equivalently)* $(c_N)_1 = 1, (c_N)_2 = 0$;
(iii) *a SMIRKN method of type* (2.9) *generated by a SMIRK method having stage order* 3 *must have* $(x_N)_{21} = 0$;
(iv) *a SMIRKN method of type* (2.10) *generated by a SMIRK method having stage order* 3 *must have* $(c_N)_1 = 0, (c_N)_2 = 1$ *and* $(x_N)_{21} = 1/6$;
(v) *the maximum stage order of a s-stage MIRKN method generated by a SMIRK method is min*$(s, 3)$.

Proof. (i), (ii) and (v) are an immediate consequence of Theorem 6 and the fact that $c_N = c$. In the case of stage order 3, if the IRKN method generated by a SMIRK method is mono-implicit in standard form (with the exception of $(x_N)_{21}$ all elements on the first two rows of X_N are necessarily zero) and of the type (2.9) with $A_N = X_N + v_N \bar{b}_N^{\mathrm{T}}$, the restriction of the stage order conditions $A_N e = c_N^2/2$ and $A_N c_N = c_N^3/6$ to the first two rows, leads for both possibilities given in (ii) to the common property that $(x_N)_{21} = 0$. Similarly, if the generated SMIRKN has stage order 3 and is of type (2.10) with $A_N = X_N + w_N b_N^{\mathrm{T}}$, then the restriction of both stage order conditions to the first two rows immediately leads to (iv). □

For practical purposes it is important to impose stability conditions on the obtained MIRKN methods. More in particular, it is natural to require that they are at least P-stable [15]. For completeness, we first recall some definitions regarding the linear stability of IRK and IRKN methods.

Definition 8 (*Lambert* [14]). The (linear) stability function of an IRK method characterized by (c, A, b), is

$$R(z) = 1 + zb^{\mathrm{T}}(I - zA)^{-1}e = \frac{|I - z(A - eb^{\mathrm{T}})|}{|I - zA|}. \tag{2.18}$$

When applied to the scalar test equation $y' = \lambda y$, a MIRK method can be written as $y_{n+1} = R(h\lambda)y_n$.

Definition 9 (*Van der Houwen et al.* [25]). The (linear) stability function of an IRKN method characterized by $(c_N, A_N, \bar{b}_N, b_N)$, is the 2×2 matrix function

$$M(z) = \begin{bmatrix} 1 + z\bar{b}_N^{\mathrm{T}}(I - zA_N)^{-1}e & 1 + z\bar{b}_N^{\mathrm{T}}(I - zA_N)^{-1}c_N \\ zb_N^{\mathrm{T}}(I - zA_N)^{-1}e & 1 + zb^{\mathrm{T}}(I - zA_N)^{-1}c_N \end{bmatrix}. \tag{2.19}$$

For the scalar test equation $y'' = -\lambda^2 y$, the MIRKN method reduces to

$$\begin{bmatrix} y_{n+1} \\ y'_{n+1} \end{bmatrix} = M(-h^2\lambda^2) \begin{bmatrix} y_n \\ y'_n \end{bmatrix}.$$

The polynomial equation

$$r^2 + \operatorname{Tr} M(-h^2\lambda^2)\, r + \det M(-h^2\lambda^2) = 0$$

is called the characteristic equation of the method for the second-order test equation $y'' = -\lambda^2 y$.

Definition 10. An IRKN method is called P-stable if for all real $z < 0$, the two (complex conjugate) eigenvalues of $M(z)$ fall on the unit circle in the complex plane. This is equivalent to with the two conditions

$$\det M(z) = 1 \text{ and } (\operatorname{Tr} M(z))^2 \leqslant 4 \qquad \forall z < 0. \tag{2.20}$$

It should be remarked that in the literature, one does not see Definition 10 for P-stability. An alternative definition is given in [15].

3. The generation of P-stable SMIRKN methods by SMIRK methods

In this section we consider the specific problem of the generation of P-stable SMIRKN methods by SMIRK methods. Our aim is to express the conditions of mono-implicitness and P-stability of the

IRKN method in terms of the characteristics of the underlying IRK method solely. The following lemma will help to set up existence conditions for the case whereby a SMIRKN method of type (2.9) is generated.

Lemma 11. *A s-stage SMIRK method that generates a SMIRKN method of type* (2.9) *is characterized by vectors b, v and a strictly lower triangular matrix X which satisfy*

$$b^{\mathrm{T}}X^{m+2}v=0 \quad \forall m\in\{0,1,2,\ldots\}. \tag{3.1}$$

Proof. From Eq. (2.15) in which P is replaced by the identity matrix, namely,

$$X_N=[X+(v-v_N)b^{\mathrm{T}}][X+vb^{\mathrm{T}}],$$

and the fact that $(x_N)_{ij}=0$ for all $1\leqslant i\leqslant j\leqslant s$, one obtains the following expressions for $(v_N)_i$ ($i=1,2,\ldots,s$):

$$(v_N)_i=v_i+\frac{(Xv)_i\,b_j+(X^2)_{ij}}{(b^{\mathrm{T}}v)\,b_j+(b^{\mathrm{T}}X)_j} \quad \forall i,j\colon\ 1\leqslant i\leqslant j\leqslant s. \tag{3.2}$$

Clearly, $(X^2)_{ij}=0$ for all $1\leqslant i\leqslant j+1\leqslant s$ and $(b^{\mathrm{T}}X)_s=0$. Furthermore, we can assume that $b_s\neq 0$, since otherwise

$$\bar{b}_s=(b^{\mathrm{T}}A)_s=(b^{\mathrm{T}}X)_s+(b^{\mathrm{T}}v)b_s=0,$$

showing that the number of effective stages is reduced. Therefore, (3.2) yields

$$(v_N)_i=v_i+\frac{(Xv)_i}{b^{\mathrm{T}}v},\quad i=1,2,\ldots,s, \tag{3.3}$$

whereas, for $i=1,2,\ldots,s-1$, the consistency of (3.2) implies that

$$\frac{(Xv)_i\,b_j}{(b^{\mathrm{T}}v)b_j+(b^{\mathrm{T}}X)_j}=\frac{(Xv)_i}{b^{\mathrm{T}}v},\quad \forall j=i,i+1,\ldots,s-1,$$

or, equivalently,

$$(Xv)_i\,(b^{\mathrm{T}}X)_j=0,\quad \forall j=i,i+1,\ldots,s-1 \quad (i=1,2,\ldots,s-1). \tag{3.4}$$

For each value of the index i, there are two possible ways to satisfy (3.4): either by $(Xv)_i=0$ or by $(b^{\mathrm{T}}X)_j=0$ for all $j=i,i+1,\ldots,s-1$.

Since $(Xv)_1=0$, let $k\in\{2,3,\ldots,s\}$ be the integer defined by the property that $(Xv)_i=0$ for $i=1,2,\ldots,k-1$, and $(Xv)_k\neq 0$. Notice that other components $(Xv)_i$ with $i>k$ might be zero as well. Then, for (3.4) to be fullfilled for all $i=1,2,\ldots,s-1$, one must have

$$\begin{array}{ll}(Xv)_i=0 & \text{for } i=1,2,\ldots,k-1,\\ (b^{\mathrm{T}}X)_i=0 & \text{for } i=k,k+1,\ldots,s.\end{array} \tag{3.5}$$

Hence, independent of the value of k, one has

$$\sum_{i=1}^{s}(b^{\mathrm{T}}X)_i(Xv)_i=b^{\mathrm{T}}X^2v=0. \tag{3.6}$$

Furthermore, since for $m=1,2,\dots,s$ the equality $(X^m)_{ij}=0$ is satisfied for all $\max\{i-m+1,1\} \leqslant j \leqslant s$, one finds

$$b^{\mathrm{T}}X^{m+2}v = \sum_{i,j=1}^{s} (b^{\mathrm{T}}X)_i (X^m)_{ij} (Xv)_j = 0. \tag{3.7}$$

Equalities (3.6) and (3.7) together prove the theorem. □

In addition, we remark that the value of k in (3.5) has implications on the structure of the vectors $b^{\mathrm{T}}X$ and Xv. Indeed, the upper $k-1$ components of Xv and the $s-k+1$ rightmost components of $b^{\mathrm{T}}X$ are zero, and therefore

$$X^{s-k+2}v = 0, \qquad b^{\mathrm{T}}X^k = 0^{\mathrm{T}}, \quad k \in \{2,3,\dots,s\},$$

whereby 0 denotes the null vector. In particular, if k has the lowest possible value 2, it follows that $b^{\mathrm{T}}X^2 = 0^{\mathrm{T}}$. □

We now derive similar results for the case whereby a SMIRK method generates a SMIRKN method of type (2.10).

Lemma 12. *A s-stage SMIRK method that generates a SMIRKN method of type* (2.10) *is characterized by vectors b, v and a strictly lower triangular matrix X which satisfy*

$$b^{\mathrm{T}}X^{m+1}v = 0 \quad \forall m \geqslant 0. \tag{3.8}$$

Proof. In this case, taking into account that $(X^2)_{ij}=0$ for $j \geqslant i-1$, (2.17) with P the identity matrix reduces to

$$(X_N)_{ij} = v_i(b^{\mathrm{T}}X)_j + (Xv)_i b_j + (b^{\mathrm{T}}v)v_i b_j - (w_N)_i b_j = 0, \quad \forall i,j\colon\ 1 \leqslant i \leqslant j \leqslant s.$$

As $(b^{\mathrm{T}}X)_s = 0$, and assuming again that $b_s \neq 0$, it follows in particular that

$$(w_N)_i = (Xv)_i + (b^{\mathrm{T}}v)v_i + \frac{(Xv)_i}{b^{\mathrm{T}}v}, \quad \forall i = 1,2,\dots,s,$$

whereas consistency simply requires that for all $i=1,2,\dots,s-1$,

$$v_i(b^{\mathrm{T}}X)_j = 0 \quad \forall j = i, i+1, \dots, s-1. \tag{3.9}$$

Let $k \in \{1,2,\dots,s\}$ now be the integer such that $v_1 = v_2 = \cdots = v_{k-1} = 0$ and $v_k \neq 0$. Then it follows from (3.9) that

$$\begin{aligned} v_i &= 0 \quad &&\text{for } i = 1,2,\dots,k-1, \\ (b^{\mathrm{T}}X)_i &= 0 \quad &&\text{for } i = k, k+1, \dots, s. \end{aligned} \tag{3.10}$$

As an immediate consequence of (3.10), one obtains

$$b^{\mathrm{T}}Xv = 0.$$

Note that this property also follows directly from (3.9) by choosing $j=i$ and taking the sum for i running from 1 to s. Finally, by the same argument as in the proof of Lemma 11, it is readily shown that

$$b^{\mathrm{T}}X^{m+1}v=0 \quad \forall m\in\{1,2,\ldots\}.$$

Combination of the last two results yields (3.8). It is also straightforward to show that, depending on the value of k in (3.10),

$$X^{s-k+1}v=0, \qquad b^{\mathrm{T}}X^k=0^{\mathrm{T}}, \quad k\in\{1,2,\ldots,s\}.$$

For $k=1$, the lowest possible value of k, one has $b^{\mathrm{T}}X=0^{\mathrm{T}}$. □

We now focus on the property of P-stability and its implications with respect to the underlying SMIRK method. Our first step consists in highlighting the relationship between the (linear) stability functions of, respectively, the IRK method and the IRKN method generated by it [25].

Theorem 13. *If an IRKN method is generated by an IRK method with Butcher tableau* (c,A,b) *and with stage order at least* 1, *then*

$$M(z)=R(Z) \quad \textit{with } Z=\left(\begin{bmatrix}0 & 1\\ z & 0\end{bmatrix}\right), \tag{3.11}$$

and where $R(Z)$ *is the* 2×2 *matrix function obtained by replacing the real variable* z *by the matrix* Z *in the formal series development of* $R(z)$ *in powers of* z, *i.e.*,

$$R(Z)=I_2+\sum_{j=0}^{\infty} Z^{j+1}b^{\mathrm{T}}A^je. \tag{3.12}$$

Proof. Since $Z^2=zI_2$, also $Z^{2k}=z^kI_2$ and $Z^{2k+1}=z^kZ$. Hence, we obtain on account of (3.12),

$$\begin{aligned}R(Z)&=I_2+\left(\sum_{j=0}^{\infty} z^jb^{\mathrm{T}}A^{2j}e\right)Z+\left(\sum_{j=0}^{\infty} z^{j+1}b^{\mathrm{T}}A^{2j+1}e\right)I_2\\ &=\begin{bmatrix}1+z\sum_{j=0}^{\infty} z^j\bar{b}_N^{\mathrm{T}}A_N^je & \sum_{j=0}^{\infty} z^jb^{\mathrm{T}}A^{2j}e\\ z\sum_{j=0}^{\infty} z^jb_N^{\mathrm{T}}A_N^je & 1+z\sum_{j=0}^{\infty} z^jb_N^{\mathrm{T}}A_N^jc_N\end{bmatrix},\end{aligned}$$

whereby use has been made of (2.13) and $Ae=c$. Furthermore, since

$$\sum_{j=0}^{\infty} z^jb^{\mathrm{T}}A^{2j}e=1+\sum_{j=0}^{\infty} z^{j+1}b^{\mathrm{T}}A^{2j+2}e=1+z\sum_{j=0}^{\infty} z^j\bar{b}_N^{\mathrm{T}}A_N^jc_N,$$

the stated relationship follows immediately. □

The conditions for P-stability of an IRKN method generated by an IRK method can be reformulated as conditions on the stability function of the IRK method solely.

Theorem 14. *An IRKN method generated by an IRK method is P-stable if* $|R(u)|=1$ *for all* u *on the imaginary axis.*

Proof. There exists a similarity transformation that diagonalizes the 2×2 matrix Z:

$$Z=Q^{-1}D(z)Q \quad \text{with } D(z)=\begin{bmatrix}\sqrt{z} & 0\\ 0 & -\sqrt{z}\end{bmatrix}.$$

Since $R(u)$ can be expressed as a convergent power series of u, one obtains

$$M(z)=R(Z)=R(Q^{-1}D(z)Q)=Q^{-1}R(D(z))Q$$

or

$$QM(z)Q^{-1}=R(D(z)).$$

In the same way as in the proof of Theorem 13 one can show that

$$R(D(z))=R\left(\begin{bmatrix}\sqrt{z} & 0\\ 0 & -\sqrt{z}\end{bmatrix}\right)=\begin{bmatrix}R(\sqrt{z}) & 0\\ 0 & R(-\sqrt{z})\end{bmatrix}.$$

Therefore,

$$\det M(z)=\det(QM(z)Q^{-1})=\det R(D(z))=R(\sqrt{z})R(-\sqrt{z})$$

and

$$\operatorname{Tr} M(z)=\operatorname{Tr}(QM(z)Q^{-1})=\operatorname{Tr} R(D(z))=R(\sqrt{z})+R(-\sqrt{z}).$$

Hence, P-stability requires that

$$R(\sqrt{z})R(-\sqrt{z})=1 \quad \text{and} \quad (R(\sqrt{z})+R(-\sqrt{z}))^2 \leqslant 4 \quad \forall z<0. \tag{3.13}$$

The left equality in (3.13) is equivalent to

$$R(\mathrm{i}\sqrt{|z|})R(-\mathrm{i}\sqrt{|z|})=1 \quad \forall z\in\mathbb{R}$$

or

$$|R(\mathrm{i}\sqrt{|z|})|=1 \quad \forall z\in\mathbb{R},$$

or, $|R(u)|=1$ for all u on the imaginary axis. Notice that by setting $R(\pm\mathrm{i}\sqrt{|z|})=U(|z|)\pm\mathrm{i}V(|z|)$, this equality is also equivalent to $U^2(|z|)+V^2(|z|)=1$ for all $z\in\mathbb{R}$. Consequently,

$$(R(\mathrm{i}\sqrt{|z|})+R(-\mathrm{i}\sqrt{|z|}))^2=(2\,U(|z|))^2\leqslant 4 \quad \forall z\in\mathbb{R}$$

which proves that the rightmost inequality in (3.13) is then automatically satisfied. □

The following sufficient criterion for P-stability of a IRKN method generated by a IRK method has been given by Gladwell and Thomas [11].

Theorem 15. *If the stability function $R(z)$ of an s-stage IRK method is of the form $R(z)=P(z)/P(-z)$ with P a polynomial in z of degree s, then the IRKN method that is generated from it is P-stable.*

Our next step consists in expressing the stability function $R(z)$ of a SMIRK method in terms of its defining characteristics b, X and v. The following result has been given in [16].

Theorem 16. *The stability function $R(z)$ of an s-stage SMIRK method can be written as*

$$R(z)=\frac{1-z\sum_{j=0}^{s-1} z^j\, b^{\mathrm{T}}X^j(v-e)}{1-z\sum_{j=0}^{s-1} z^j\, b^{\mathrm{T}}X^j v}. \tag{3.14}$$

On account of Theorem 14, a SMIRK method that generates a P-stable SMIRKN method, whether it is one of type (2.9) or of type (2.10), must have a stability function $R(u)$ with modulus 1 for all u on the imaginary axis. Consequently, by setting $u=\mathrm{i}t$ with $t\in\mathbb{R}$, the SMIRKN is P-stable if the equality

$$\begin{aligned}&\left|1+\sum_{j=0}^{\lfloor (s-1)/2\rfloor}(-1)^j t^{2j+2} b^{\mathrm{T}}X^{2j+1}(v-e)-\mathrm{i}t\sum_{j=0}^{\lfloor s/2\rfloor-1}(-1)^j t^{2j} b^{\mathrm{T}}X^{2j}(v-e)\right|^2\\ &\quad-\left|1+\sum_{j=0}^{\lfloor (s-1)/2\rfloor}(-1)^j t^{2j+2} b^{\mathrm{T}}X^{2j+1}v-\mathrm{i}t\sum_{j=0}^{\lfloor s/2\rfloor-1}(-1)^j t^{2j} b^{\mathrm{T}}X^{2j}v\right|^2=0\end{aligned} \tag{3.15}$$

is identically satisfied for all $t\in\mathbb{R}$. Notice that the left-hand side of (3.15) is an even polynomial in t of degree at most $2s$. Hence, the condition for P-stability of the SMIRKN method is equivalent to at most $s+1$ conditions to be satisfied by the X, b and v of the underlying SMIRK method. The condition emerging from the constant term in (3.15) (i.e., the term in t^0) is trivially satisfied. We will now show that, depending on the order of the method, more conditions out of the set induced by (3.15) are identically satisfied.

Theorem 17. *If a SMIRKN method has order $p\geqslant 2$, the term in t^{2j} on the left-hand side of* (3.15) *identically vanishes for all $1\leqslant j\leqslant\lfloor p/2\rfloor$.*

Proof. Clearly, (3.15) is the equality $|R(\mathrm{i}t)|^2-1=0$ expressed in terms of the matrix X. If, however, by means of (2.18) and an infinite series expansion for $(I-zA)^{-1}$ with $z=\mathrm{i}t$, this same equality is reexpressed in terms of the matrix A, one obtains

$$\begin{aligned}R(\mathrm{i}t)&=1+\mathrm{i}t\sum_{j=0}^{\infty}(\mathrm{i}t)^j b^{\mathrm{T}}A^j e\\ &=1-t^2\sum_{j=0}^{\infty}(-1)^j t^{2j} b^{\mathrm{T}}A^{2j+1}e+\mathrm{i}t\sum_{j=0}^{\infty}(-1)^j t^{2j} b^{\mathrm{T}}A^{2j}e.\end{aligned}$$

If the SMIRK method has order p, then in particular the order conditions

$$b^{\mathrm{T}}A^k e = \frac{1}{(k+1)!} \quad \forall k \in \{0,1,\ldots,p-1\}$$

are satisfied. Hence,

$$1 - t^2 \sum_{j=0}^{\infty} (-1)^j t^{2j} b^{\mathrm{T}} A^{2j+1} e = 1 - t^2 \sum_{j=0}^{\infty} (-1)^j \frac{t^{2j}}{(2j+2)!} + \mathcal{O}((t^2)^{\lfloor p/2 \rfloor + 1})$$
$$= \cos t + \mathcal{O}((t^2)^{\lfloor p/2 \rfloor + 1})$$

and

$$t \sum_{j=0}^{\infty} (-1)^j t^{2j} b^{\mathrm{T}} A^{2j} e = \sum_{j=0}^{\infty} (-1)^j \frac{t^{2j+1}}{(2j+1)!} + \mathcal{O}(t(t^2)^{\lfloor (p+1)/2 \rfloor})$$
$$= \sin t + \mathcal{O}((t^2)^{\lfloor (p+1)/2 \rfloor}).$$

Clearly, the given order conditions imply that

$$|R(\mathrm{i}t)|^2 = 1 + \mathcal{O}((t^2)^{\lfloor p/2 \rfloor + 1}),$$

which proves the theorem. □

We are now able to give the fundamental theorem concerning the existence of P-stable SMIRKN methods generated by SMIRK methods.

Theorem 18. *A P-stable SMIRKN method of type* (2.9) *generated by a SMIRK method can have at most order* 4 *and a P-stable SMIRKN method of type* (2.10) *generated by a SMIRK method can have at most order* 2.

Proof. In the case of a SMIRKN method of type (2.9), it is known from Lemma 11 that $b^{\mathrm{T}}X^{m+2}v = 0$ for all integer $m \geqslant 0$. Hence, the second part on the left-hand side of (3.15) reduces to a polynomial with terms solely in t^0, t^2 and t^4. Clearly, (3.15) is only identically satisfied for all $t \in \mathbb{R}$ if also the first part reduces to a polynomial in t of degree at most 4. Hence, one necessarily has that

$$b^{\mathrm{T}}X^{m+2}e = 0 \quad \forall m \in \{0,1,2,\ldots\}. \tag{3.16}$$

from which one obtains

$$R(z) = \frac{1 - zb^{\mathrm{T}}(v-e) - z^2 b^{\mathrm{T}}X(v-e)}{1 - zb^{\mathrm{T}}v - z^2 b^{\mathrm{T}}Xv}.$$

Since the numerator and denominator of $R(z)$ are both of degree not greater than 2, this rational function is at most an order 4 approximation to $\exp(z)$ (see, e.g., [14, p. 233]), from which the first part of the theorem follows. If, moreover, the maximum order 4 is attained, the stability function $R(z)$ is the R_{22} Padé approximant of $\exp(z)$.

Likewise, it follows from Lemma 12 and the P-stability condition (3.15) that for methods of the type (2.10) the numerator and denominator of $R(z)$ are at most linear in z, giving the second part of the theorem. □

It should be remarked that similar arguments do not apply to the case of nonstandard MIRKN methods generated by SMIRK methods and so far we have not been able to find for the order of such methods an upper bound that is strictly lower than the trivial bound of twice the number of stages.

4. Examples of P-stable SMIRKN methods

A complete classification of the SMIRKN methods which are generated by SMIRK methods and which are of order at most 4, can be done with the help of symbolic computing packages. Since it is impossible to describe all these methods in a concise way, we have taken the option to consider here only certain families of SMIRK methods which have been reported on recently in the literature [1, 21, 10] and to generate from them P-stable SMIRKN methods of the type (2.9). To that aim, we shall require that (3.15) be identically satisfied for all real t, which ensures the P-stability of the generated IRKN method. Furthermore, we shall require that a $k \in \{2,3,\dots,s\}$ exists such that

$$\begin{aligned} (Xv)_i &= 0 \quad \text{for } i=1,2,\dots,k-1, \\ (b^{\mathrm{T}}X)_i &= 0 \quad \text{for } i=k,k+1,\dots,s. \end{aligned} \tag{4.1}$$

Then the choice

$$(v_N)_i = v_i + \frac{(Xv)_i}{b^{\mathrm{T}}v}, \quad i=1,2,\dots,s, \tag{4.2}$$

ensures that the generated IRKN method is a SMIRKN method.

4.1. SMIRKN methods with one stage

For the class of one-stage SMIRK 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 free parameter and $x_{11} = 0$. Choosing $c_1 = \frac{1}{2}$ gives the unique one-stage SMIRK method of order 2, i.e., the midpoint rule [1]. Since $X = 0$, condition (4.1) is trivially satisfied and according to (4.2) the choice $(v_N)_1 = v_1$ has to be made. On the other hand, the P-stability condition (3.15) which reduces to

$$|1 - \mathrm{i}tb_1(v_1 - 1)|^2 - |1 - \mathrm{i}tb_1 v_1|^2 = 0 \quad \forall t \in \mathbb{R}$$

is identically satisfied if and only if $v_1 = \frac{1}{2}$. Hence, the only P-stable one-stage SMIRKN method generated by the given family of SMIRK methods has order 2 and is characterized by the tableau

$$\begin{array}{c|c|c|c} \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \hline & & & \\ & & & \frac{1}{2} \\ & & & 1 \end{array}$$

The stability function of the SMIRK method is the R_{11} Padé approximant of $\exp(z)$ and the characteristic equation of the SMIRKN method is given by

$$r^2 - 2\,\frac{1-h^2\lambda^2/2}{1+h^2\lambda^2/2}\,r + 1 = 0.$$

4.2. SMIRKN methods with two stages

There exists a one-parameter family of second-order, two-stage SMIRK methods [21], characterized by $X=0, c_1=v_1=0, b_2=1-b_1$ and $c_2=v_2=1/(2b_1-2)$, where b_1 is the free parameter. For $b_1=\frac{1}{2}$ the method reduces to the trapezoidal rule, which has stage order 2.

As $X=0$, it follows from Theorem 17 that (3.15) is, irrespective of the value of b_1, identically satisfied. Also (4.1) is trivially satisfied and consequently, the choice $(v_N)_1=v_1$, $(v_N)_2=v_2$, leads to the one-parameter family of P-stable SMIRKN methods characterized by the tableau

0	0	0	0	0
$\frac{1}{2(1-b_1)}$	$\frac{1}{2(1-b_1)}$	0	0	0
			$\frac{1}{2}b_1$	$\frac{1}{2}-\frac{1}{2}b_1$
			b_1	$1-b_1$

Since for any b_1, the stability function $R(z)$ of the SMIRK method is the R_{11} Padé approximant of $\exp(z)$, the order cannot be increased by giving b_1 an appropriate value. Burrage et al. [1] have reported a one-parameter family of two-stage third-order SMIRK methods. However, the P-stability condition (3.15) cannot be fulfilled for any particular choice of the parameters present.

4.3. SMIRKN methods with three stages

Burrage et al. [1] cite a family of third-order SMIRK methods with stage order at least 2, characterized by the tableau

1	1	0	0	0
c_2	$c_2(2-c_2)$	$c_2(c_2-1)$	0	0
c_3	v_3	$\frac{c_3(c_3-2c_2)+v_3(2c_2-1)}{2(1-c_2)}$	$\frac{v_3+c_3(c_3-2)}{2(c_2-1)}$	0
		$\frac{6c_2c_3-3c_3-3c_2+2}{6(c_2-1)(c_3-1)}$	$\frac{3c_3-1}{6(c_2-1)(c_2-c_3)}$	$\frac{3c_2-1}{6(c_3-1)(c_3-c_2)}$

where c_2, c_3 and v_3 are the free parameters, with the restriction that 1, c_2 and c_3 are all different. Stage order 3 is obtained when $c_2=0$ and $v_3=c_3^2(3-2c_3)$.

Since $(Xv)_1=0$ and $(b^{\mathrm{T}}X)_3=0$, condition (4.1) can be realized if either $(Xv)_2=x_{21}v_1=0$ or $(b^{\mathrm{T}}X)_2=b_3x_{32}=0$. Since $v_1=1$ and $c_2\neq 1$, the first possibility is equivalent with $c_2=0$, whereas the second possibility, assuming $b_3\neq 0$ (otherwise the number of stages would be reduced), is equivalent to $v_3=c_3(2-c_3)$.

On account of Theorem 17 and the property $X^3 = 0$, the polynomial on the left-hand side of (3.15) reduces to the single term

$$(b^{\mathrm{T}}Xe)[b^{\mathrm{T}}X(2v-e)]t^4.$$

Hence, the generated method will be P-stable if at least one of the factors $b^{\mathrm{T}}Xe$ and $b^{\mathrm{T}}X(2v-e)$ is zero. When $c_2 = 0$, $b^{\mathrm{T}}Xe = 0$ is equivalent to $v_3 = c_3$, whereas $b^{\mathrm{T}}X(2v-e) = 0$ is equivalent to $c_3(1-c_3) = 0$. The latter possibility is excluded since by assumption $c_3 \neq 1$ and $c_3 \neq c_2 = 0$. When $v_3 = c_3(2-c_3)$, it is easy to verify that $b^{\mathrm{T}}Xe = b^{\mathrm{T}}X(2v-e) = -\frac{1}{6}$, and P-stability cannot be realized.

In conclusion, the only P-stable SMIRKN methods that can be generated from the given family of SMIRK methods, are those corresponding to the choice

$$c_2 = 0, \qquad v_3 = c_3.$$

With the help of (4.2) one obtains the following characterizing tableau:

$$\begin{array}{c|c|c|ccc}
1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
c_3 & c_3^2 & 0 & \frac{c_3(c_3-1)}{12} & \frac{c_3(1-c_3)}{12} & 0 \\
\hline
 & & & \frac{2c_3-1}{12(c_3-1)} & \frac{4c_3-1}{12c_3} & -\frac{1}{12c_3(c_3-1)} \\
 & & & \frac{3c_3-2}{6(c_3-1)} & \frac{3c_3-1}{6c_3} & -\frac{1}{6(c_3-1)c_3}
\end{array}$$

whereas the characteristic equation reads

$$r^2 - 2\,\frac{1 - 5/12h^2\lambda^2 + 1/144h^4\lambda^4}{1 + 1/12h^2\lambda^2 + 1/144h^4\lambda^4}\,r + 1 = 0.$$

It can be verified that for $c_3 = \frac{1}{2}$ a three-stage, order 4, stage order 3 SMIRKN method is obtained.

4.4. SMIRKN methods with four stages

The present authors have constructed a four-parameter family of four-stage SMIRK methods of order at least 4 and having stage order 2. The parameters are c_3, c_4, v_3 and x_{43} also denoted by θ, with the restriction that $c_3 \neq c_4, c_3 \notin \{0, \frac{1}{2}, 1\}$ and $c_4 \notin \{0, 1\}$. The family is characterized by the tableau:

$$\begin{array}{c|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 \\
c_3 & v_3 & c_3 - \frac{1}{2}c_3^2 - \frac{1}{2}v_3 & \frac{1}{2}c_3^2 - \frac{1}{2}v_3 & 0 & 0 \\
c_4 & \frac{\omega}{c_3 - 3c_3^2 + 2c_3^3} & \frac{\tau}{c_3 - 3c_3^2 + 2c_3^3} & \frac{\rho}{c_3 - 3c_3^2 + 2c_3^3} & \theta & 0 \\
\hline
 & & \frac{\delta}{12c_3c_4} & \frac{\beta}{12(1-c_3)(1-c_4)} & \frac{2c_4-1}{12c_3(c_4-c_3)(1-c_3)} & \frac{1-2c_3}{12c_4(c_4-c_3)(1-c_4)}
\end{array}$$

where

$$\omega = -3c_3^2c_4 + 2c_3^3c_4 + 3c_3c_4^2 - 2c_3c_4^3 - 6c_3^2\theta + 24c_3^3\theta - 30c_3^4\theta + 12c_3^5\theta + c_4v_3 - 3c_4^2v_3 + 2c_4^3v_3,$$

$$\tau = \tfrac{1}{2}(2c_3c_4 - 3c_3^2c_4 + 2c_3^3c_4 - 4c_3c_4^2 + 3c_3^2c_4^2 - 2c_3^3c_4^2 + 2c_3c_4^3 - 2c_3\theta$$
$$+ 14c_3^2\theta - 34c_3^3\theta + 34c_3^4\theta - 12c_3^5\theta - c_4v_3 + 3c_4^2v_3 - 2c_4^3v_3),$$

$$\rho = \tfrac{1}{2}(3c_3^2c_4 - 2c_3^3c_4 - 2c_3c_4^2 - 3c_3^2c_4^2 + 2c_3^3c_4^2 + 2c_3c_4^3 + 4c_3^2\theta$$
$$- 18c_3^3\theta + 26c_3^4\theta - 12c_3^5\theta - c_4v_3 + 3c_4^2v_3 - 2c_4^3v_3),$$

$$\delta = 1 - 2(c_3 + c_4) + 6c_3c_4, \qquad \beta = 3 - 4(c_3 + c_4) + 6c_3c_4.$$

By choosing $v_3 = c_3^2(3 - 2c_3)$, one obtains the three-parameter family of four-stage SMIRK methods of order at least 4 and having stage order 3, which has been reported on by Burrage et al. [1].

Since $(Xv)_1 = (Xv)_2 = (b^TX)_4 = 0$, (4.1) is satisfied if either $(Xv)_3 = 0$ which is equivalent to $v_3 = c_3^2$ or $(b^TX)_3 = 0$ which is equivalent to $\theta = 0$ (b_4 is assumed different from zero).

On account of Theorem 17 and the property $X^3 = 0$, the polynomial on the left-hand side of (3.15) reduces to the single term

$$(b^TX^2e)[b^TX^2(2v - e)]t^6.$$

If $\theta = 0$, then $X^2 = 0$ and the generated SMIRKN method is P-stable. If $v_3 = c_3^2$ the only nonzero element of X^2 is $(X_2)_{41} = \theta(2c_3 - c_3^2 - v_3)/2$ and since $b_4 \neq 0$ and $v_1 = 0$, P-stability can only be ensured if $v_3 = 2c_3 - c_3^2$, hence if $c_3 = 0$ or $c_3 = 1$. These values being excluded, the P-stable SMIRKN methods that can be generated from the given family of SMIRK methods correspond to the choice $\theta = 0$ and they are characterized by the tableau:

$$\begin{array}{c|c|c|cccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 \\
c_3 & c_3^2 & 0 & -\frac{1}{12}c_3^2 + \frac{1}{12}v_3 & \frac{1}{12}c_3^2 - \frac{1}{12}v_3 & 0 & 0 \\
c_4 & c_4^2 & 0 & -\kappa & \kappa & 0 & 0 \\
\hline
 & & & \frac{\xi}{24c_3c_4} & \frac{\psi}{24(c_3-1)(c_4-1)} & \frac{2c_4-1}{24c_3(c_3-c_4)(c_3-1)} & \frac{2c_3-1}{24c_4(c_3-c_4)(c_4-1)} \\
 & & & \frac{\delta}{12c_3c_4} & \frac{\beta}{12(1-c_3)(1-c_4)} & \frac{2c_4-1}{12c_3(c_4-c_3)(1-c_3)} & \frac{1-2c_3}{12c_4(c_4-c_3)(1-c_4)}
\end{array}$$

with

$$\xi = 8c_3c_4 - 2(c_3 + c_4) + 1,$$

$$\psi = 4c_3c_4 - 2(c_3 + c_4) + 1,$$

$$\kappa = \frac{c_4(2c_3^3c_4 + 3c_3^2 - 3c_3^2c_4 - 2c_3c_4 + 2c_3c_4^2 - 2c_4^2v_3 - v_3 + 3c_4v_3 - 2c_3^3)}{12c_3(c_3 - 1)(2c_3 - 1)},$$

and whereby $c_3 \notin \{0, \frac{1}{2}, 1\}$, $c_4 \notin \{0, 1\}$ and v_3 are the free parameters. All these SMIRKN methods have order 4 and stage order at least 2. Choosing $v_3 = c_3^2(3 - 2c_3)$ results in SMIRKN methods with stage order 3.

As a final example, we consider the generation of four-stage SMIRKN methods corresponding with two coinciding c_i values. They cannot directly be obtained as special cases of the previous example. Instead, they can be generated from the so-called double-stride, four-stage, order 4, stage order 2 SMIRK methods which have been constructed and classified by the present authors [10]. One of these families of SMIRK methods is defined by the tableau

0	0	0	0	0	0
1	1	0	0	0	0
$\frac{1}{2}$	$\frac{t}{q}$	$\frac{3q-4t}{8q}$	$\frac{q-4t}{8q}$	0	0
$\frac{1}{2}$	$\frac{3s}{2-3q}$	$\frac{-10-24t+12s+27q}{24(-2+3q)}$	$\frac{2-24t+12s+9q}{24(-2+3q)}$	$\frac{2(-1+3t+3s)}{3(-2+3q)}$	0
		$\frac{1}{6}$	$\frac{1}{6}$	q	$\frac{2}{3}-q$

where s, t and $q \notin \{0, \frac{2}{3}\}$ are the free parameters. Proceeding in exactly the same way as before, one can first show that (4.1) is satified if either $s = \frac{1}{3} - t$ or $q = 4t$. Only the first possibility is compatible with the requirement of P-stability and the corresponding two-parameter family of SMIRKN methods is characterized by the tableau

0	0	0	0	0	0	0
1	1	0	0	0	0	0
$\frac{1}{2}$	$\frac{1}{4}$	0	$\frac{4t-q}{48q}$	$-\frac{4t-q}{48q}$	0	0
$\frac{1}{2}$	$\frac{1}{4}$	0	$\frac{(-2+12t-3q)}{48(-2+3q)}$	$-\frac{(-2+12t-3q)}{48(-2+3q)}$	$\frac{2(-1+3t+3s)}{3(-2+3q)}$	0
			$\frac{1}{6}$	0	$\frac{q}{2}$	$\frac{1}{3}-\frac{q}{2}$
			$\frac{1}{6}$	$\frac{1}{6}$	q	$\frac{2}{3}-q$

The stage order is at least 2; stage order 3 can only be obtained when $q = 2t$.

5. Conclusions

In this paper we have considered the conditions to be imposed on a SMIRK method to guarantee that it will generate a P-stable SMIRKN method. These conditions imply the existence of some order barriers for the methods considered. The requirement, however, that the generated MIRKN method be in standard form is, from the practical point of view, not relevant. As a matter of fact, since MIRKN methods can be easily converted to SMIRKN methods through a relabelling of the stages, it would be of interest to investigate the more general problem of generating MIRKN methods from SMIRK methods. Although in this case there are indications that methods of order higher than 4 might exist, we have at present, not been able to prove any order barriers.

Finally, it should be mentioned that numerical experiments have been carried out with some of the P-stable SMIRKN methods given in the present paper. Their behaviour is in complete agreement with the results we obtained in earlier experiments [23, 24] and which are related to SMIRKN methods for which the c_i's take integer values.

Acknowledgements

We express our gratitude to the (unknown) referees for their comments and suggestions. We also thank one of the referees for pointing out a way to make our original proof of Theorem 18 considerably shorter.

References

[1] K. Burrage, F.H. Chipman, P.H. Muir, Order results for mono-implicit Runge–Kutta methods, SIAM J. Numer. Anal. 31 (1994) 876–891.
[2] J.C. Butcher, The Numerical Analysis of Ordinary Differential Equations, Wiley, Toronto, 1987.
[3] J.R. Cash, High-order P-stable formulae for the numerical integration of periodic initial value problems, Numer. Math. 37 (1981) 355–370.
[4] J.R. Cash, Efficient P-stable methods for periodic initial value problems, BIT 24 (1984) 248–252.
[5] J.R. Cash, A. Singhal, Mono-implicit Runge–Kutta formulae for the numerical integration of stiff differential systems, IMA J. Numer. Anal. 2 (1982) 211–227.
[6] M.M. Chawla, M.A. Al-Zanaidi, M.S. Al-Sahhar, Stabilized fourth order extended methods for the numerical solution of ODEs, Internat. J. Comput. Math. 52 (1994) 99–107.
[7] M.M. Chawla, M.A. Al-Zanaidi, M.S. Al-Sahhar, A class of stabilized extended one-step methods for the numerical solution of ODEs, Comput. Math. Appl. 29 (1995) 79–84.
[8] M.M. Chawla, A.A. Karaballi, M.S. Al-Sahhar, Extended double-stride L-stable methods for the numerical solution of ODEs, Comput. Math. Appl. 31 (1996) 1–6.
[9] M.M. Chawla, P.S. Rao, High accuracy P-stable methods for $y'' = f(t, y)$, IMA J. Numer. Anal. 5 (1985) 215–220.
[10] H. De Meyer, T. Van Hecke, G. Vanden Berghe, M. Van Daele, Multistride L-stable Fourth-Order methods for the numerical solution of ODEs, Comput. Math. Appl. 32 (1996) 1–8.
[11] I. Gladwell, R. Thomas, A-stable methods for second-order differential systems and their relation to Padé approximants, in: P.R. Graves-Morris, E. Saff, R.S. Varga (Eds.), Rational Approximation and Interpolation, Lecture Notes in Mathematics, vol. 1105, Springer, Berlin, 1984, pp. 419–430.
[12] E. Hairer, S.P. Nørsett, G. Wanner, Solving Ordinary Differential Equations I, Nonstiff Problems, Springer, Heidelberg, 1987.
[13] I.B. Jacques, Extended one-step methods for the numerical solution of ordinary differential equations, Internat. J. Comput. Math. 29 (1989) 247–255.
[14] J.D. Lambert, Numerical Methods for Ordinary Differential Systems, the Initial Value Problem, Wiley, Chichester, 1991.
[15] J.D. Lambert, I.A. Watson, Symmetric multistep methods for periodic initial value problems, J. Inst. Math. Appl. 18 (1976) 189–202.
[16] P.H. Muir, W.H. Enright, Relationships among some classes of IRK methods and their stability functions, BIT 27 (1987) 403–423.
[17] R.M. Thomas, Efficient fourth order P-stable formulae, BIT 24 (1987) 599–614.
[18] R.M. Thomas, Efficient sixth order methods for nonlinear oscillation problems, BIT 28 (1988) 898–903.
[19] R.M. Thomas, High order, P-stable methods for nonlinear oscillation problems, Numerical Analysis Report No. 221, University of Manchester/UMIST, 1992.
[20] R.S. Usmani, R.P. Agarwal, An A-stable extended trapezoidal rule for the numerical integration of ordinary differential equations, Comput. Math. Appl. 11 (1985) 1183–1191.
[21] W.M.G. van Bokhoven, Efficient higher order implicit one-step methods for integration of stiff differential equations, BIT 20 (1980) 34–43.

[22] M. Van Daele, G. Vanden Berghe, H. De Meyer, A general theory of stabilized extended one-step methods for ODEs, Internat. J. Comput. Math. 60 (1996) 253–263.

[23] T. Van Hecke, M. Van Daele, G. Vanden Berghe, H. De Meyer, A mono-implicit Runge–Kutta–Nyström Modification of the Numerov method, J. Comput. Appl. Math. 78 (1997) 161–178.

[24] T. Van Hecke, M. Van Daele, G. Vanden Berghe, H. De Meyer, P-stable mono-implicit Runge–Kutta–Nyström modifications of the Numerov method, in: Lecture Notes in Computer Science, vol. 1196, Proc. 1st Internat. Workshop WNAA'96, Rousse, Bulgaria, Springer, Berlin, 1997, pp. 537–545.

[25] P.J. Van der Houwen, B.P. Sommeijer, Nguyen Huu Cong, Stability of collocation-based Runge–Kutta–Nyström methods, BIT 31 (1991) 469–481.