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A Practical Approach for the Derivation of Algebraically Stable Two-Step Runge-Kutta Methods

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Abstract. We describe an algorithm, based on a new strategy recently proposed by Hewitt and Hill in the context of general linear methods, for the construction of algebraically stable two-step Runge-Kutta methods. Using this algorithm we obtained a complete characterization of algebraically stable methods with one and two stages.

Keywords: ordinary differential equations, two-step Runge-Kutta methods, general linear methods, G-stability, algebraic stability.

AMS Subject Classification: 65L05; 65L06; 65L20.

1 Introduction

Consider the initial-value problem for ordinary differential equations (ODEs)

$$\begin{cases} y'(t) = f\big(y(t)\big), & t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{1.1}$$

where the function $f : \mathbb{R}^m \to \mathbb{R}^m$ is assumed to be sufficiently smooth and $y_0 \in \mathbb{R}^m$ is a given initial value.

The nonlinear stability analysis of general linear methods (GLMs) for the numerical solution of the problem (1.1) is subject of several recent papers (compare, for instance, [7, 16, 17, 18, 19]). In this paper we focus our attention on the subclass of two-step Runge-Kutta (TSRK) methods [21, 22], whose nonlinear stability properties are object of some preliminary results obtained in [9, 10, 11]. In fact, in these papers an optimization-based numerical approach has been used to derive the coefficients of algebraically stable TSRK methods. Because of the purely numerical nature of this approach, the coefficients of the corresponding methods are not expressed in rational form, but they are provided with a certain number of correct digits. As a consequence, the derived methods satisfy a slightly weaker condition than that of algebraic stability, i.e. they are ε-algebraically stable methods. This concept has been recently introduced in [20], to which we refer for more details. In order to find algebraically stable TSRK methods whose coefficients are expressed in rational form, in this paper we use the approach proposed by Hewitt and Hill in [17].

The paper is organized as follows. In Sections 2 and 3 WE recall the main concepts regarding TSRK methods and algebraic stability for GLMs. In Section 4 we describe the derivation of an algorithm for the construction of algebraically stable TSRK methods based on the approach of Hewitt and Hill [17]. Then in Sections 5 and 6 TSRK methods with one and two stages are analized in details. Finally, some conclusions are reported in Section 7.

2 Two-Step Runge-Kutta Methods

For the numerical solution of (1.1) we consider the general class of TSRK methods which on the uniform grid

$$I_h = \big\{t_n = t_0 + nh,\ n = 0, 1, \dots, N,\ Nh = T - t_0\big\},$$

are defined by the formulas

$$\begin{cases} Y_i^{[n]} = (1 - u_i)y_{n-1} + u_i y_{n-2} + h\displaystyle\sum_{j=1}^{s}\big(a_{ij} f\big(Y_j^{[n]}\big) + b_{ij} f\big(Y_j^{[n-1]}\big)\big), \\ y_n = (1 - \vartheta)y_{n-1} + \vartheta y_{n-2} + h\displaystyle\sum_{j=1}^{s}\big(v_j f\big(Y_j^{[n]}\big) + w_j f\big(Y_j^{[n-1]}\big)\big), \end{cases} \tag{2.1}$$

$i = 1, 2, \dots, s$. Here, y_n is an approximation of order p to $y(t_n)$ and $Y_i^{[n]}$ are approximations of stage order q to $y(t_{n-1} + c_i h)$, where $y(t)$ is the solution to (1.1) and $c = [c_1, \dots, c_s]^T$ is the abscissa vector. TSRK methods (2.1) can be represented by the abscissa vector c and the following table of its coefficients

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v^T & w^T \end{array} = \begin{array}{c|ccc|ccc} u_1 & a_{11} & \cdots & a_{1s} & b_{11} & \cdots & b_{1s} \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u_s & a_{s1} & \cdots & a_{ss} & b_{s1} & \cdots & b_{ss} \\ \hline \vartheta & v_1 & \cdots & v_s & w_1 & \cdots & w_s \end{array}.$$

In this paper we focus on methods (2.1) with order p and stage order $q = p$. It was proved in [8] that this condition is satisfied if and only if

$$\widehat{C}_k = 0, \qquad C_k = 0, \quad k = 1, 2, \dots, p, \tag{2.2}$$

where

$$\widehat{C}_k = \frac{1}{k!} - \frac{(-1)^k}{k!}\vartheta - \frac{v^T c^{k-1}}{(k-1)!} - \frac{w^T(c-e)^{k-1}}{(k-1)!},$$
$$C_k = \frac{c^k}{k!} - \frac{(-1)^k}{k!}u - \frac{Ac^{k-1}}{(k-1)!} - \frac{B(c-e)^{k-1}}{(k-1)!}.$$

Here $e = [1, \dots, 1]^T \in \mathbb{R}^s$ and c^k denotes componentwise exponentiation.

It is well known that TSRK methods (2.1) are a subclass of GLMs which assume the form

$$\left[\begin{array}{c} Y^{[n]} \\ \hline z^{[n]} \end{array}\right] = \left[\begin{array}{c|c} \mathbf{A}\otimes\mathbf{I} & \mathbf{U}\otimes\mathbf{I} \\ \hline \mathbf{B}\otimes\mathbf{I} & \mathbf{V}\otimes\mathbf{I} \end{array}\right] \left[\begin{array}{c} hf(Y^{[n]}) \\ \hline z^{[n-1]} \end{array}\right], \tag{2.3}$$

with $z^{[n]} \in \mathbb{R}^r$, $\mathbf{A} \in \mathbb{R}^{s\times s}$, $\mathbf{U} \in \mathbb{R}^{s\times r}$, $\mathbf{B} \in \mathbb{R}^{r\times s}$, $\mathbf{V} \in \mathbb{R}^{r\times r}$ and

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix}, \qquad hf(Y^{[n]}) = \begin{bmatrix} hf(Y_1^{[n]}) \\ \vdots \\ hf(Y_s^{[n]}) \end{bmatrix}, \qquad z^{[n]} = \begin{bmatrix} z_1^{[n]} \\ \vdots \\ z_r^{[n]} \end{bmatrix},$$

where $\mathbf{I}$ denotes the identity matrix of dimension m and '$\otimes$' stands for Knonecker product of matrices. It can be verified that TSRK methods (2.1) can be represented as GLMs (2.3) with coefficient matrices $\mathbf{A}$, $\mathbf{U}$, $\mathbf{B}$, and $\mathbf{V}$, defined by

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|ccc} A & e-u & u & B \\ \hline v^T & 1-\vartheta & \vartheta & w^T \\ 0 & 1 & 0 & 0 \\ I & 0 & 0 & 0 \end{array}\right], \tag{2.4}$$

and vector $z^{[n]} = [y_{n-1},\ y_{n-2},\ hf(Y^{[n-1]})]^T \in \mathbb{R}^{s+2}$. Since a GLM (2.3) is zero-stable if the coefficient matrix $\mathbf{V}$ is power bounded, the zero-stability condition for TSRK methods (2.1) is

$$-1 < \vartheta \le 1. \tag{2.5}$$

We will also focus on the family of TSRK methods with $\vartheta = 0$, $u = 0$, whose GLM representation reduces to

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} A & e & B \\ \hline v^T & 1 & w^T \\ I & 0 & 0 \end{array}\right]. \tag{2.6}$$

We observe that such methods are automatically zero-stable.

3 Algebraic Stability of General Linear Methods

The GLM (2.3) is said to be algebraically stable, if there exist a real, symmetric and positive definite matrix $\mathbf{G} \in \mathbb{R}^{r\times r}$ and a real, diagonal and positive definite matrix $\mathbf{D} \in \mathbb{R}^{s\times s}$ such that the matrix $\mathbf{M} \in \mathbb{R}^{(s+r)\times(s+r)}$ defined by

$$\mathbf{M} = \left[\begin{array}{c|c} \mathbf{D}\mathbf{A} + \mathbf{A}^T\mathbf{D} - \mathbf{B}^T\mathbf{G}\mathbf{B} & \mathbf{D}\mathbf{U} - \mathbf{B}^T\mathbf{G}\mathbf{V} \\ \hline \mathbf{U}^T\mathbf{D} - \mathbf{V}^T\mathbf{G}\mathbf{B} & \mathbf{G} - \mathbf{V}^T\mathbf{G}\mathbf{V} \end{array}\right] \tag{3.1}$$

is nonnegative definite. The significance of this definition follows from the result proved by Butcher [5, 6, 15], that for preconsistent and non-confluent GLMs (2.3), i.e. methods with distinct abscissas c_i, $i = 1, 2, \ldots, s$, algebraic stability is equivalent to G-stability. We refer to [5, 6, 15] for the definition of G-stability. We recall that a GLM is preconsistent if there exists a vector $\mathbf{q}_0$ (called preconsistency vector) such that

$$\mathbf{U}\mathbf{q}_0 = e, \qquad \mathbf{V}\mathbf{q}_0 = \mathbf{q}_0,$$

compare [21].

In general, it is quite difficult to check if a given GLM is algebraically stable, and even more difficult to construct new classes of GLMs which are algebraically stable. In our search for such methods we will use the fact, proved in [4], that for a preconsistent and algebraically stable GLM (2.3) the matrices $\mathbf{G}$ and $\mathbf{D}$ are not independent but related by the equation

$$\mathbf{D}e = \mathbf{B}^T\mathbf{G}\mathbf{q}_0, \tag{3.2}$$

where $\mathbf{q}_0$ is the preconsistency vector.

We will write $\mathbf{M} \geq 0$ if the matrix $\mathbf{M}$ is nonnegative definite. It was observed by Hewitt and Hill [16, 17] that the analysis of the nonnegative definiteness of the matrix $\mathbf{M}$ can be simplified by the use of the result proved by Albert [1]. This result states that the matrix $\mathbf{M}$ given by

$$\mathbf{M} = \left[\begin{array}{c|c} \mathbf{M}_{11} & \mathbf{M}_{12} \\ \hline \mathbf{M}_{12}^T & \mathbf{M}_{22} \end{array}\right]$$

satisfies $\mathbf{M} \geq 0$ if and only if

$$\mathbf{M}_{11} \geq 0, \qquad \mathbf{M}_{22} - \mathbf{M}_{12}^T\mathbf{M}_{11}^+\mathbf{M}_{12} \geq 0, \qquad \mathbf{M}_{11}\mathbf{M}_{11}^+\mathbf{M}_{12} = \mathbf{M}_{12}, \tag{3.3}$$

or, equivalently,

$$\mathbf{M}_{22} \geq 0, \qquad \mathbf{M}_{11} - \mathbf{M}_{12}\mathbf{M}_{22}^+\mathbf{M}_{12}^T \geq 0, \qquad \mathbf{M}_{22}\mathbf{M}_{22}^+\mathbf{M}_{12}^T = \mathbf{M}_{12}^T. \tag{3.4}$$

Here, $\mathbf{A}^+$ stands for the Moore–Penrose pseudoinverse of the matrix $\mathbf{A}$. We refer to [13, 14] for the definition of this notion.

Although the criteria based on Albert theorem can be used to verify if specific examples of GLMs are algebraically stable, these criteria are not very practical to search for algebraically stable GLMs which depend on some unknown parameters, unless some suitable simplifications are introduced. This will be object of the following section.

4 Construction of Algebraically Stable TSRK Methods

In order to find algebraically stable TSRK methods, we use the approach proposed recently by Hewitt and Hill in [17]. This approach consists in enforcing algebraic stability through the following steps:

(a) fix the matrix $\mathbf{G} = \mathbf{I}$;

(b) ensure that $\mathbf{D} = \mathbf{B}^T\mathbf{q}_0 > 0$;

(c) ensure that $\mathbf{M}_{22} = \mathbf{I} - \mathbf{V}^T\mathbf{V} \geq 0$;

(d) impose the condition

$$\mathbf{R} := \mathbf{D}\mathbf{A} + \mathbf{A}^T\mathbf{D} - \mathbf{B}^T\mathbf{B} - (\mathbf{D}\mathbf{U} - \mathbf{B}^T\mathbf{V})(\mathbf{I} - \mathbf{V}^T\mathbf{V})^+(\mathbf{D}\mathbf{U} - \mathbf{B}^T\mathbf{V})^T = 0.$$

We observe that conditions (c) and (d) are obtained from (3.4) considering the second inequality as an equality, and neglecting the third equality, which is automatically satisfied when $\mathbf{M}_{22}$ is invertible.

The following results will lead to the reformulation of the above conditions in the case of TSRK methods (2.1).

Theorem 1. *Algebraically stable TSRK methods* (2.1) *with* $\mathbf{G} = \mathbf{I}$ *satisfy*

$$v_i > 0, \quad i = 1, 2, \ldots, s.$$

Proof. We recall that for a TSRK method the preconsistency vector is $\mathbf{q}_0 = [1, 1, 0, 0, \ldots, 0]^T \in \mathbb{R}^{s+2}$ (compare [21]). Then, taking into account that from (2.4) $\mathbf{B}^T = [v,\ 0,\ \mathbf{I}]$, condition (3.2) implies that

$$\mathbf{D}e = v. \tag{4.1}$$

The thesis now follows from the condition (b). □

Theorem 2. *An algebraically stable TSRK method* (2.1) *with* $\mathbf{G} = \mathbf{I}$ *and not reducing to* (2.6) *is non-consistent.*

Proof. We prove that condition (c) is equivalent to $\vartheta = 1$, $w = 0$. In fact, from (2.4), we have

$$\mathbf{M}_{22} = \mathbf{I} - \mathbf{V}^T\mathbf{V} = \begin{bmatrix} -(1-\vartheta)^2 & -\vartheta(1-\vartheta) & -(1-\vartheta)w^T \\ -\vartheta(1-\vartheta) & 1-\vartheta^2 & -\vartheta w^T \\ -(1-\vartheta)w & -\vartheta w & I - ww^T \end{bmatrix}.$$

We define

$$\mathbf{N} = \begin{bmatrix} 0 & \alpha(1+\vartheta) & 0 \\ \frac{\alpha}{1+\vartheta} & 2\alpha\vartheta - w^T w & 0 \\ \beta w & -\beta w & I \end{bmatrix},$$

with

$$\alpha = 1 - \vartheta, \qquad \beta = -\frac{\alpha(\vartheta+1)}{(\vartheta+1)w^T w - \alpha\theta^2},$$

and

$$\mathbf{X} = \begin{bmatrix} -\frac{w^T w}{\alpha} & \vartheta & w^T \\ -\frac{\vartheta^2}{1+\vartheta} & \vartheta & w^T \\ -w & -w & I \end{bmatrix},$$

whose inverse is

$$\mathbf{X}^{-1}=\left[\begin{array}{ccc}\beta & -\beta & 0\\ \frac{\beta\left(\vartheta^2-(1+\vartheta)w^Tw\right)}{(1+\vartheta)(w^Tw+\vartheta)} & -\frac{\beta\vartheta w^Tw}{\alpha(w^Tw+\vartheta)} & -\frac{w^T}{w^Tw+\vartheta}\\ \frac{\beta\vartheta(1+2\vartheta)}{(1+\vartheta)(w^Tw+\vartheta)}w & -\frac{\beta(w^Tw+\alpha\vartheta)}{\alpha(w^Tw+\vartheta)}w & I-\frac{ww^T}{w^Tw+\vartheta}\end{array}\right].$$

Then, the matrix $\mathbf{M}_{22}$ can be obtained by the similarity transformation

$$\mathbf{M}_{22}=\mathbf{X}^{-1}\mathbf{N}\mathbf{X},$$

and its spectrum is $\sigma(\mathbf{M}_{22})=\sigma(\mathbf{N})=\{\lambda_1,\lambda_2,\lambda_3\}$, where λ_1 and λ_2 are the roots of the quadratic polynomial

$$p(\lambda)=\lambda^2-(2\alpha\vartheta-w^Tw)\lambda-\alpha^2, \tag{4.2}$$

and $\lambda_3=1$ with multiplicity s. Then, condition $\mathbf{M}_{22}\geq 0$ is equivalent to

$$\lambda_1\geq 0, \quad \text{and} \quad \lambda_2\geq 0. \tag{4.3}$$

This condition is of course satisfied if $\vartheta=1$ and $w=0$, because it leads to $p(\lambda)=\lambda^2$. Vice versa, let us suppose that (4.3) is satisfied and, by contradiction, we suppose $\vartheta\neq 1$. Then, $-\alpha^2<0$ and, by Descartes' rule of signs, the polynomial (4.2) has a positive root and a negative one. This contradicts (4.3), so it is $\vartheta=1$ and, in correspondence of this value, the polynomial (4.2) assumes the form $p(\lambda)=\lambda(\lambda+w^Tw)$, whose roots are $\lambda_1=0$ and $\lambda_2=-w^Tw$. Therefore, in force of condition (4.3), it is $w=0$. Then, the third condition in (3.4) provides that

$$\left[\begin{array}{c}\frac{1}{2}v^T(u-e)\\ v^T(e-\frac{u}{2})\\ 0\end{array}\right]=0,$$

which implies $v=0$. Thus, the consistency condition $\widehat{C}_1=0$ in (2.2) is not satisfied. □

As a consequence of Theorem 2, in our search for algebraically stable methods we have to abandon TSRK methods of the form (2.4), and consider only the reduced form (2.6) corresponding to $\vartheta=0$ and $u=0$.

Theorem 3. *An algebraically stable TSRK method* (2.1) *with* $\mathbf{G}=\mathbf{I}$, $\vartheta=0$ *and* $u=0$, *satisfies* $w=0$.

Proof. We prove that condition (c) is equivalent to $w=0$. From the formulation of $\mathbf{V}$ in (2.6) we obtain

$$\mathbf{M}_{22}=\mathbf{I}-\mathbf{V}^T\mathbf{V}=\left[\begin{array}{cc}0 & -w^T\\ -w & I-ww^T\end{array}\right].$$

We define

$$\mathbf{N}=\left[\begin{array}{cc}-w^Tw & (1-w^Tw)w^T\\ 0 & I\end{array}\right], \quad \mathbf{X}=\left[\begin{array}{cc}w^Tw & w^T\\ -w & I\end{array}\right],$$

whose inverse is

$$\mathbf{X}^{-1} = \frac{1}{2w^T w} \begin{bmatrix} 1 & -w^T \\ w & 2w^T w I - ww^T \end{bmatrix}.$$

The matrix $\mathbf{M}_{22}$ can be obtained by the similarity transformation

$$\mathbf{M}_{22} = \mathbf{X}^{-1}\mathbf{N}\mathbf{X}.$$

Thus, $\sigma(\mathbf{M}_{22}) = \sigma(\mathbf{N}) = \{1, -w^T w\}$, where the eigenvalue 1 has multiplicity s. It follows that $\mathbf{M}_{22}$ is nonnegative definite if and only if $w = 0$. $\square$

Theorem 3 leads to searching for algebraically stable TSRK methods (2.1) within the family

$$\begin{cases} Y_i^{[n]} = y_{n-1} + h \sum_{j=1}^{s} \left(a_{ij} f\left(Y_j^{[n]}\right) + b_{ij} f\left(Y_j^{[n-1]}\right)\right), \\ y_n = y_{n-1} + h \sum_{j=1}^{s} v_j f\left(Y_j^{[n]}\right). \end{cases} \tag{4.4}$$

The following result provides representation formulas for the coefficients of a non-confluent algebraically stable TSRK method with $\mathbf{G} = \mathbf{I}$, of order and stage order s. We recall that a GLM is non-confluent if $c_i \neq c_j$, $i \neq j$.

Theorem 4. *The coefficients of a non-confluent TSRK method* (4.4) *with* $p = q = s$ *satisfy the following representation formulas:*

$$v_i = \int_0^1 L_i(x)\, dx, \tag{4.5}$$

where $L_i(x)$ *are the fundamental Lagrange polynomials,* $i = 1, 2, \ldots, s$, *with respect to* $\{c_1, c_2, \ldots, c_s\}$, *and*

$$A = (C - BE)\widetilde{C}^{-1}, \tag{4.6}$$

where $E = \begin{bmatrix} e & c-e & \cdots & (c-e)^{s-1} \end{bmatrix}$, $C = \begin{bmatrix} c & c^2/2 & \cdots & c^s/s \end{bmatrix}$, $\widetilde{C} = \begin{bmatrix} e & c & \cdots & c^{s-1} \end{bmatrix}$.

Proof. For the family of methods (4.4), order conditions $\widehat{C}_k = 0$, $k = 1, \ldots, s$, in (2.2) assume the form

$$v^T c^{k-1} = \frac{1}{k}, \quad k = 1, 2, \ldots, s,$$

which are the order conditions for interpolatory quadrature rules with weights v_i and nodes c_i. Therefore, the weights v_i can be expressed as integrals (4.5).

We next compute the coefficient matrix A from stage order conditions $C_k = 0$, $k = 1, 2, \ldots, s$, in (2.2), which are equivalent to

$$A\widetilde{C} = C - BE.$$

Hence, as the method is non-confluent, the matrix $\widetilde{C}$ is nonsingular and the representation formula (4.6) holds. □

The advancing formula in (4.4) is completely determined in the case $p = q = s$, since the expression of the weights v_i is given in (4.5). Thus, the unknown coefficients of algebraically stable methods (4.4) are only the entries of the matrices A and B. These unknown matrices have to be derived by imposing condition (d), i.e. $\mathbf{R} = 0$, and the representation formula (4.6).

Theorem 5. *For methods of type* (4.4)*, the condition* $\mathbf{R} = 0$ *is equivalent to*

$$a_{ij} = \begin{cases} (l_{ij} - v_j a_{ji})/v_i, & j > i, \\ l_{ij}/2v_i, & j = i, \end{cases} \tag{4.7}$$

with $\mathbf{L} = \mathbf{I} + \mathbf{D}(ee^T + BB^T)\mathbf{D}$.

Proof. Taking into account representation (2.6) with $w = 0$ and (4.1), we have

$$(I - \mathbf{V}^T\mathbf{V})^+ = \begin{bmatrix} 0 & 0 \\ 0 & I \end{bmatrix},$$

$$\mathbf{B}^T\mathbf{B} = I + vv^T = I + \mathbf{D}ee^T\mathbf{D}, \quad \mathbf{D}\mathbf{U} - \mathbf{B}^T\mathbf{V} = \begin{bmatrix} 0 & \mathbf{D}B \end{bmatrix}.$$

Then, the matrix $\mathbf{R}$ assumes the form

$$\mathbf{R} = \mathbf{D}A + A^T\mathbf{D} - \mathbf{I} - \mathbf{D}(ee^T + BB^T)\mathbf{D}. \tag{4.8}$$

Since $\mathbf{R}$ is a symmetric matrix, the matrix equation $\mathbf{R} = 0$ is equivalent to a linear system of $s(s+1)/2$ scalar equations. The thesis is obtained by solving this system with respect to the upper triangular part of the matrix A. □

The results proved in this section lead to the following algorithm for the construction of algebraically stable TSRK methods (2.1) of order $p = q = s$:

(i) fix the matrix $\mathbf{G} = \mathbf{I}$;

(ii) put $\vartheta = 0$ and $u = w = 0$, i.e. consider the class of TSRK methods (4.4);

(iii) compute v_i from (4.5), and ensure $v_i > 0$, $i = 1, 2, \ldots, s$, finding the region of $\mathbb{R}^s$ to which the vector c of the nodes has to belong;

(iv) compute a_{ij}, $j \geq i$, as a function of B through (4.7);

(v) derive a_{ij}, $j < i$, as a function of B through the lower triangular part of (4.6) and partly compute the remaining s^2 parameters, i.e. the entries of the matrix B, by solving the nonlinear system of $s(s+1)/2$ equations arising from the upper triangular part of (4.6).

The remaining free parameters can be exploited, for instance, in order to reduce the error constant of the method, or the contributions of high order terms as in [12].

We observe as the above algorithm combines steps (a)–(d) of Hewitt and Hill approach [17] with order conditions (2.2): step (ii) corresponds to (c); (iii) stands for (b), together with $\widehat{C}_k = 0$, $k = 1, 2, \ldots, s$; (iv) matches with (d), and (v) corresponds to $C_k = 0$, $k = 1, 2, \ldots, s$.

5 Analysis of Methods with $s = 1$

By applying the algorithm derived in the previous section, we obtain a one parameter family of algebraically stable TSRK methods (4.4) with $p = q = s = 1$ and real-valued coefficients depending on the free parameters $c_1 \geq 1/2$, having

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v & w \end{array} = \begin{array}{c|c|c} 0 & 1 + c_1 + \sqrt{2c_1 - 1} & -1 - \sqrt{2c_1 - 1} \\ \hline 0 & 1 & 0 \end{array}.$$

The spectrum of the matrix $\mathbf{M}$ contains $\lambda_0 = 0$ with multiplicity 2 and $\lambda_1 = 1 + 2c_1 + 2\sqrt{2c_1 - 1}$, whose plot as a function of c_1 is reported in Figure 1.

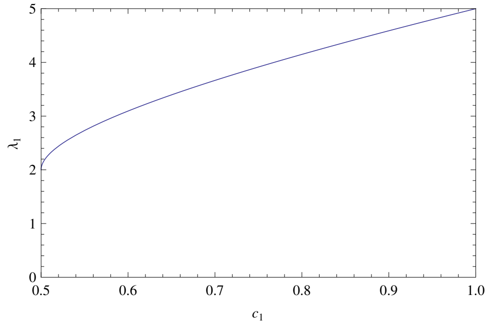

Figure 1. Plot of the eigenvalue λ_1 of the matrix $\mathbf{M}$ for algebraically stable TSRK methods (4.4) with $p = q = s = 1$.

We observe that in correspondence of the value $c_1 = 1/2$, a further order condition is satisfied, i.e. $\widehat{C}_2 = 0$. Therefore, we obtain the following algebraically stable TSRK method of order $p = 2$ and stage order $q = 1$.

$$\begin{array}{c|c|c} u & A & B \\ \hline \vartheta & v & w \end{array} = \begin{array}{c|c|c} 0 & \frac{3}{2} & -1 \\ \hline 0 & 1 & 0 \end{array}$$

6 Analysis of Methods with $s = 2$

We apply the algorithm derived in Section 4, in order to derive algebraically stable methods within the class (4.4) of order 2 and stage order 2. Step (iii) provides that

$$v_1 = \frac{1 - 2c_2}{2(c_1 - c_2)}, \qquad v_2 = \frac{2c_1 - 1}{2(c_1 - c_2)},$$

with the condition

$$\left(c_1 > \frac{1}{2} \text{ and } c_2 < \frac{1}{2}\right) \quad \text{or} \quad \left(c_1 < \frac{1}{2} \text{ and } c_2 > \frac{1}{2}\right). \tag{6.1}$$

We derive the matrix A from steps (iv) and (v), obtaining

$$
\begin{aligned}
a_{11} &= -\frac{d_1^2 - 2d_2d_1 + (b_{11}^2 + b_{12}^2 + 2)d_2^2}{2(d_1 - d_2)d_2},\\
a_{12} &= \frac{d_1(-(d_2-1)^2 + 4b_{21}(-d_1 + b_{11}d_2 + d_2 + 2) + 4b_{22}(b_{12}d_2 + 2))}{4(d_1 - d_2)d_2},\\
a_{21} &= \frac{-(d_2+1)^2 + 8b_{22} + 4b_{21}(-d_1 + d_2 + 2)}{4(d_1 - d_2)},\\
a_{22} &= \frac{(b_{21}^2 + b_{22}^2 + 2)d_1^2 - 2d_2d_1 + d_2^2}{2d_1(d_1 - d_2)},
\end{aligned}
$$

where $d_1 = 2c_1 - 1$ and $d_2 = 2c_2 - 1$. As a result of step (v), we obtain

$$
\begin{aligned}
b_{21} &= -\frac{4d_1 + \sqrt{-2d_1^2(\alpha_0 + \alpha_1 b_{22} + 2d_1^2 b_{22}^2)}}{2d_1^2},\\
b_{12} &= \frac{\sqrt{2(d_1 - d_2)^2 {d_2}^2 (17 + 3d_1d_2)^2 (\alpha_0 + \alpha_1 b_{22} + 2d_1^2 b_{22}^2)} + \beta_0 + \beta_1 b_{22}}{4{d_2}^2(8\,(-2 + d_2) + d_1(-9 - 2d_1d_2 + {d_2}^2))},\\
b_{11} &= \frac{\gamma_0 - 8d_1b_{22} + \gamma_1 b_{21} + (\gamma_2 - 4d_1d_2b_{22})b_{12}}{4d_2(2 + b_{21}d_1)},
\end{aligned}
$$

with

$$
\begin{aligned}
\alpha_0 &= -8 + d_1(-1 + 2d_1) - 2d_1(2 + d_1)d_2 + (2 + d_1)d_2^2,\\
\alpha_1 &= 4d_1(2 + d_1 - d_2),\\
\beta_0 &= -2d_2(d_1 - d_2)(-2 + d_2 + d_1(1 + d_2(-6 + d_1 + d_2))),\\
\beta_1 &= -2d_1d_2(32 + d_2 + d_1(1 + d_2(d_1 + d_2))),\\
\gamma_0 &= d_1(d_2(d_1 + d_2) + 1) + d_2,\\
\gamma_1 &= 4d_1(d_1 - d_2 - 2), \quad \gamma_2 = -4d_2(d_1 - d_2 + 2).
\end{aligned}
$$

Since $b_{21} \neq -2/d_1$ (otherwise the denominator of b_{11} vanishes), the coefficients b_{12} and b_{21} are real if and only if

$$\alpha_0 + \alpha_1 b_{22} + 2d_1^2 b_{22}^2 < 0, \tag{6.2}$$

and $17 + 3d_1d_2 = 0$, i.e.

$$c_1 = \frac{3c_2 - 10}{6c_2 - 3}. \tag{6.3}$$

We observe that, in force of (6.3), condition (6.1) reduces to $c_2 \neq 1/2$.

Thus algebraically stable TSRK methods (4.4) with $p = q = s = 2$ and real-valued coefficients form a two-parameter family of methods with coefficients depending on the free parameters $c_2 \neq 1/2$ and $b_{22} \in \mathbb{R}$, satisfying (6.2), with coefficients A, B and v derived previously. The region of acceptable values for these parameters is reported in Figure 2.

The spectrum of matrix $\mathbf{M}$ of algebraic stability corresponding to $b_{22} = 0$ is $\{\lambda_0, \lambda_1, \lambda_2\}$, where $\lambda_0 = 0$ has multiplicity 3, and λ_1, λ_2 are depicted in

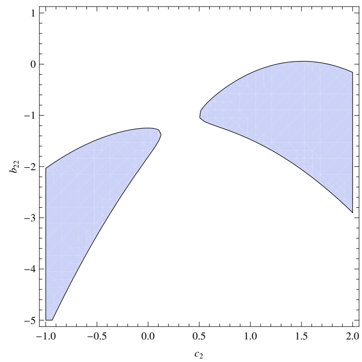

Figure 2. Region of algebraic stability for TSRK methods (4.4) with $p = q = s = 2$ and real-valued coefficients.

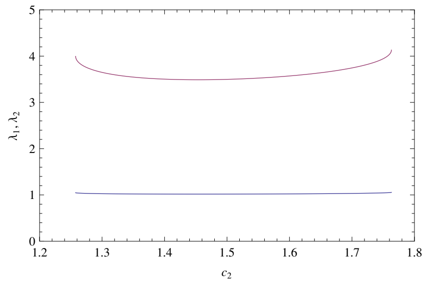

Figure 3. Plot of the eigenvalues λ_1 and λ_2 of the matrix $\mathbf{M}$ for algebraically stable TSRK methods (4.4) with $p = q = s = 2$.

Figure 3 as functions of c_2, which varies in the interval of admissible values obtainable from Figure 2. For instance, if we choose $c_2 = 3/2$, we obtain $c_1 = -11/12$ and

$$A = \begin{bmatrix} \frac{3541-82\sqrt{34}}{696} & \frac{-119+24\sqrt{34}}{696} \\ \frac{-525+82\sqrt{34}}{986} & \frac{6(109-2\sqrt{34})}{493} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{-41+\sqrt{34}}{12} & -\frac{29}{12} \\ \frac{12-\sqrt{34}}{17} & 0 \end{bmatrix}, \quad v = \begin{bmatrix} \frac{12}{29} & \frac{17}{29} \end{bmatrix}^T.$$

The analysis carried out in this section is exhaustive for two-stage methods, as it is made clear by the following order barrier.

Theorem 6. *The maximum attainable order of convergence for two-stage algebraically stable TSRK methods* (4.4) *with* $\mathbf{G} = \mathbf{I}$ *is two.*

Proof. We remind (compare [21, 22]) that the order conditions which guarantee order $p = 3$, with possibly $q \neq p$, are

$$\widehat{C}_1 = \widehat{C}_2 = \widehat{C}_3 = 0, \qquad C_1 = 0, \qquad (v^T + w^T)C_2 = 0.$$

Performing the steps (i)–(iv) of the algorithm and further imposing the conditions $\widehat{C}_3 = 0$, $C_1 = 0$, we obtain that $(v^T + w^T)C_2 = -2$, which is a contradiction. This concludes the proof. □

Future work will address the construction of higher order algebraically stable TSRK methods with $\mathbf{G} = \mathbf{I}$ and $s \geq 3$, or with possibly $\mathbf{G} \neq \mathbf{I}$, by extending the results of [2, 3].

7 Conclusions

We described an algorithm for the practical construction of algebraically stable TSRK methods. This approach is based on the recent work of Hewitt and Hill [17]. The TSRK methods with one and two stages have been completely analized.

The derived algebraically stable methods are fully implicit and their implementation requires the solution of nonlinear systems of dimension $m \cdot s$, where m is the dimension of the problem and s the number of stages. Although this is less efficient than for algorithms based for instance on SIRK or Gear methods [15, 23], the methods derived in this paper have stage order equal to the order and as a result do not suffer from order reduction phenomenon [6]. Therefore they are appropriate for stiff differential systems discussed for example in [15].

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