Stability issues in multivalue numerical methods for ordinary differential equations

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Abstract—We describe the derivation of highly stable general linear methods for the numerical solution of initial value problems for systems of ordinary differential equations. In particular we describe the construction of explicit Nordsiek methods and implicit two step Runge Kutta methods with stability properties determined by quadratic stability functions. We aim for methods which have wide stability regions in the explicit case and which are A- and L-stable in the implicit one case. We moreover describe the construction of algebraically stable and G-stable two step Runge Kutta methods. Examples of methods are then provided.

Keywords—algebraic stability, quadratic stability, G-stability, general linear methods, two step Runge Kutta methods

I. Introduction

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

$$\begin{cases} y'(t) = f(y(t)), & t \in [t_0, T], \\ y(t_0) = y_0, \end{cases} \tag{1}$$

where the function $f : \mathbb{R}^d \to \mathbb{R}^d$ is sufficiently smooth. Concerning the numerical solution of the problem (1), recent work in the literature has been devoted to the derivation of highly stable multivalue or general linear numerical methods which posses also high stage order, with the aim of providing accurate numerical solutions and avoiding order reduction phenomenon. Consider a uniform grid $t_n = t_0 + nh$, $n = 0, 1, \ldots, N$, $h = (T - t_0)/N$. A general linear method (GLM) with coefficient matrices $\mathbf{A} \in \mathbb{R}^{s\times s}$, $\mathbf{U} \in \mathbb{R}^{s\times r}$, $\mathbf{B} \in \mathbb{R}^{r\times s}$, $\mathbf{V} \in \mathbb{R}^{r\times r}$ and abscissa vector $\mathbf{c} \in \mathbb{R}^s$, assumes the form

$$\left[\begin{array}{c} Y^{[n]} \\ \hline z^{[n]} \end{array}\right] = \left[\begin{array}{c|c} \mathbf{A}\otimes\mathbf{I} & \mathbf{U}\otimes\mathbf{I} \\ \hline \mathbf{B}\otimes\mathbf{I} & \mathbf{V}\otimes\mathbf{I} \end{array}\right] \left[\begin{array}{c} hf(Y^{[n]}) \\ \hline z^{[n-1]} \end{array}\right], \tag{2}$$

$n = 1, 2, \ldots, N$ with

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

$$z^{[n]} = \begin{bmatrix} z_1^{[n]} \\ \vdots \\ z_r^{[n]} \end{bmatrix},$$

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where s is the number of internal stages, r is the number of input and output approximations, $\mathbf{I}$ denotes the identity matrix of dimension d and '$\otimes$' stands for Knonecker product of matrices. For the analog formulation of general linear methods approximating second order differential problems, compare [46], [47], [50], [60] and references therein.

GLMs (2) depend on a plenty of free parameters, thus there are a lot of degrees of freedom to gain strong stability properties together with high accuracy. In particular in the papers [51]–[53], [56], [57], [63], [73], A- and L- stable continuous collocation-based methods, belonging to the family of two-step Runge-Kutta (TSRK) formulas introduced in [73], [74], were constructed and analyzed. A very useful property for the practical derivation of highly stable methods, e.g. A- and L- stable in the implicit case and methods with large stability regions in the explicit one, is the property of inherent quadratic stability, which guarantees that the stability properties of the method depend on a quadratic polynomial. The approach of inherent quadratic stability has been used in the papers [4], [35], [73] in the implicit case, and in papers [5], [27], [28] in the explicit one case.

Similar methods were investigated in [50], [64] for second order differential equations, in [34], [38], [41], [44], [45] for Volterra integral equations, in [22], [24] for Volterra integro-differential equations and in [23] for fractional differential equations. Different approaches to the construction of continuous TSRK methods outside collocation have been presented in literature in the papers [2], [3], [75]. As regards the nonlinear stability properties of GLMs, it has beel subject of several papers, see for instance [8], [16], [36], [37], [68]–[71].

In this paper we consider some classes of GLMs and describe several approaches for the derivation of highly stable methods. In particular in Section II we describe the constuction of highly stable GLMs within the classes of implicit two step Runge Kutta (TSRK) methods and explicit Nordsiek methods, with inherent quadratic stability. In Section III we describe the construction of algebraically stable GLMs within the class of TSRK methods. Finally in Section IV some conclusions are drawn.

II. Quadratic stability

In order to analyze the linear stability properties of the GLM (2) we apply the method to the linear test equation

$$y' = \xi y, \quad t \geq 0, \tag{3}$$

where $\xi \in \mathbb{C}$, it follows that the stability properties of (38) with respect to (3) are determined by the stability matrix $\mathbf{M}(z)$

defined by

$$\mathbf{M}(z) = \mathbf{V} + z\mathbf{B}(\mathbf{I_s} - z\mathbf{A})^{-1}\mathbf{U}, \tag{4}$$

where $z = h\xi \in \mathbb{C}$. We also define the stability function $p(\omega, z)$ as the characteristic polynomial of $\mathbf{M}(z)$, i.e.,

$$p(\omega, z) = \det\Big(\omega I_{s+2} - \mathbf{M}(z)\Big). \tag{5}$$

This is a polynomial of degree r with respect to ω whose coefficients are rational functions with respect to z. In the following subsections we describe the practical derivation of methods with inherent quadratic stability (IQS), which is defined as follows:

Definition 2.1: The GLM method (2) has inherent quadratic stability (IQS) if there exists a matrix $\mathbf{X} \in \mathbb{R}^{r\times r}$ such that

$$\mathbf{BA} \equiv \mathbf{XB} \quad \text{and} \quad \mathbf{BU} \equiv \mathbf{XV} - \mathbf{VX}. \tag{6}$$

Here, the relation $\mathbf{P} \equiv \mathbf{Q}$ means that the matrices $\mathbf{P}$ and $\mathbf{Q}$ are identical with the exception of the first two rows.

As we will see in Subsection II-A for Nordsieck methods and in the Subsection 66 for TSRK methods, IQS condition leads to a quadratic stability polynomial. The constructed methods will be order p and stage order $q = p$ for which the stability properties are determined by quadratic stability functions. Since $p = q$ these methods do not suffer from the order reduction phenomenon. We recall the definitions of order and stage order for the GLM (2). Assume that

$$z_i^{[n-1]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_{n-1}) + O(h^{p+1}),\ i = 1, \ldots, r. \tag{7}$$

The method (2) has stage order q and order p if

$$Y_i^{[n]} = y(t_{n-1} + c_i h) + O(h^{q+1}), \quad i = 1, \ldots, s,$$

and

$$z_i^{[n]} = \sum_{k=0}^{p} q_{ik} h^k y^{(k)}(t_n) + O(h^{p+1}), \quad i = 1, \ldots, r,$$

for the same parameters q_{ik}.

A. Explicit Nordsieck methods with quadratic stability

In this subsection we focus on explicit GLMs in Nordsieck form, where the matrix $\mathbf{A}$ is strictly lower triangular and matrix $\mathbf{V}$ have this form:

$$\mathbf{A} = \begin{bmatrix} 0 & & & & \\ a_{21} & 0 & & & \\ a_{31} & a_{32} & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} & 0 \end{bmatrix}, \tag{8}$$

$$\mathbf{V} = \begin{bmatrix} 1 & v_{12} & v_{13} & \cdots & v_{1r} \\ 0 & 0 & v_{23} & \cdots & v_{2r} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & & \ddots & v_{r-1,r} \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}, \tag{9}$$

so that the considered GLM is also zero-stable, i.e. the matrix $\mathbf{V}$ is power bounded.

A GLM in Nordsieck form is given by (2), where $z_i^{[n]}$ is an approximation of order p to the component $h^{i-1}y^{(i-1)}(t_n)$ of the Nordsieck methods, i.e. if

$$z_i^{[n-1]} = h^{i-1}y^{(i-1)}(t_{n-1}) + O\left(h^{p+1}\right),$$

then

$$z_i^{[n]} = h^{i-1}y^{(i-1)}(t_n) + O\left(h^{p+1}\right),$$

i=1,. . . ,r.

Put

$$\mathbf{q}_k := [q_{1k}, \ldots, q_{rk}]^T.$$

Since for the subclass of GLM (2) we are considering here, $z_i^{[n-1]}$ represents an approximation of order p to the Nordsieck vector $z(t_{n-1}, h)$, the vectors $\{\mathbf{q}_0, \ldots, \mathbf{q}_{r-1}\}$ represent the canonical basis of $\mathbb{R}^r$, usually indicated as $\{\mathbf{e}_1, \ldots, \mathbf{e}_r\}$. Let us introduce also

$$\mathbf{w}(z) = \sum_{k=0}^{p} \mathbf{q}_k z^k,$$

and

$$e^{\mathbf{c}z} = [e^{c_1 z} e^{c_1 z} \ldots e^{c_s z}]^T.$$

The following theorems gives the order conditions (70) for GLM in Nordsieck form. For a deeper investigation and complete proof compare [5], [6], [15], [18], [27], [28], [73], [80], while for further references on order conditions of GLMs compare [7], [32].

Theorem 2.1: The GLM (2) in Nordsieck form has order p and stage order $q = p$, with $p = q = r - 1 = s - 1$ if and only if

$$e^{\mathbf{c}z} = z\mathbf{A}e^{\mathbf{c}z} + \mathbf{U}Z + O(z^{p+1}), \tag{10}$$

$$e^{z}Z = z\mathbf{B}e^{\mathbf{c}z} + \mathbf{V}Z + O(z^{p+1}), \tag{11}$$

where $e^{\mathbf{c}z} = [\ e^{c_1 z} \quad e^{c_2 z} \quad \cdots \quad e^{c_s z}\ ]^T$ and $Z = [\ 1 \quad z \quad \cdots \quad z^{r-1}\ ]^T$.

Theorem 2.2: Assume that $z^{[n-1]}$ satisfies (70). Then the GLM (2) in Nordsieck form has order p and stage order $q = p - 1$ if and only if

$$\begin{aligned} e^{\mathbf{c}z} = \quad & z\mathbf{A}e^{\mathbf{c}z} + \mathbf{U}\mathbf{w}(z) \\ & + \left(\frac{\mathbf{c}^p}{p!} - \frac{\mathbf{A}\mathbf{c}^{p-1}}{(p-1!)} - \mathbf{U}\mathbf{q}_p\right) z^p + O(z^{p+1}), \end{aligned} \tag{12}$$

$$e^{z}\mathbf{w}(z) = z\mathbf{B}e^{\mathbf{c}z} + \mathbf{V}\mathbf{w}(z) + O(z^{p+1}). \tag{13}$$

By suitable series expansion of order conditions (10)-(38) and (12)-(13), algebraic conditions on the coefficient matrices can been derived, see for example [5], [18], [27]. In particular, let us consider the case $p = q = s$ and $r = s+1$. Let partition $\mathbf{B}$, $\mathbf{V}$, and $\mathbf{E}_{p+1}$ as follows:

$$\mathbf{B} = \left[\begin{array}{c} \mathbf{b}^T \\ \hline \widetilde{\mathbf{B}} \end{array}\right], \mathbf{V} = \left[\begin{array}{c|c} 1 & \mathbf{v} \\ \hline \mathbf{0} & \widetilde{\mathbf{V}} \end{array}\right], \mathbf{E}_{p+1} = \left[\begin{array}{c|c} 1 & E_p^T \\ \hline \mathbf{0} & \mathbf{E}_p \end{array}\right]$$

where $\mathbf{b}^T$ stands for the first row of $\mathbf{B}$ and $\mathbf{0}$ stands for vector or matrix of appropriate dimension. We can obtain the following result.

Theorem 2.3: [4] Assume that $c_i \neq c_j$, for any $i \neq j$ and that the GLM (2) with $r = s + 1$ has order and stage order $p = q = s$. Then we have this representation of the matrices $\mathbf{U}$ and $\mathbf{B}$:

$$\mathbf{U} = \mathbf{C}_{p+1} - \mathbf{A}\mathbf{C}_{p+1}\mathbf{K}_{p+1}, \tag{14}$$

$$\mathbf{b}^T = (E_p^T - \mathbf{v})\mathbf{C}_p^{-1}, \tag{15}$$

and

$$\widetilde{\mathbf{B}} = (\mathbf{E}_p - \widetilde{\mathbf{V}})\mathbf{C}_p^{-1}. \tag{16}$$

In the case $p = r = s = q + 1$ a similar result can be proved, compare [5].

In order to simplify the search for methods with good stability properties, we require that the method possesses the quadratic stability property, i.e. the stability function defined by (5) assumes this expression:

$$p(w, z) = w^{r-2}\left(w^2 - p_{r-1}(z)w + p_{r-2}(z)\right), \tag{17}$$

where

$$\begin{aligned} p_{r-1}(z) &= 1 + p_{r-1,1}z + p_{r-1,2}z^2 + \cdots + p_{r-1,s}z^s, \\ p_{r-2}(z) &= p_{r-2,1}z + p_{r-2,2}z^2 + \cdots + p_{r-2,s}z^s. \end{aligned} \tag{18}$$

A sufficient condition for the quadratic stability is IQS condition of Definition 2.1. In [4], [27] the following theorem was proved, asserting that IQS condition leads to quadratic stability.

Theorem 2.4: Assume that the GLM (2) with matrices $\mathbf{A}$ and $\mathbf{V}$ as in (8)-(9) has IQS. Then the stability function of the method assumes the form (17) with $p_{r-1}(z)$ and $p_{r-2}(z)$ given by (39).

The structure of matrix $\mathbf{X}$ appearing in (6) is analyzed in the following theorems [5], [27].

Theorem 2.5: For a GLM (2) with $p = r = s$ and $q = s-1$, the most general matrix $\mathbf{X}$ satisfying conditions (6) is of the form:

$$\mathbf{X} = \left[\begin{array}{cccccc|c} x_{1,1} & x_{1,2} & x_{1,3} & \cdots & x_{1,s-1} & & x_{1,s} \\ x_{2,1} & x_{2,2} & x_{2,3} & \cdots & x_{1,s-1} & & x_{2,s} \\ \hline 0 & 1 & 0 & \cdots & 0 & & q_{3s} \\ 0 & 0 & 1 & \cdots & 0 & & q_{4s} \\ \vdots & \vdots & \vdots & \ddots & \vdots & & \\ 0 & 0 & 0 & \cdots & 1 & & q_{ss} \end{array}\right],$$

Theorem 2.6: For a GLM of type (2) with $p = q = s$ and $r = s+1$, the most general matrix $\mathbf{X}$ satisfying conditions (6) is of the form:

$$\mathbf{X} = \left[\begin{array}{cccccc|c} x_{1,1} & x_{1,2} & x_{1,3} & \cdots & x_{1,r-1} & & x_{1,r} \\ x_{2,1} & x_{2,2} & x_{2,3} & \cdots & x_{2,r-1} & & x_{2,r} \\ \hline 0 & 1 & 0 & \cdots & 0 & & x_{3,r} \\ 0 & 0 & 1 & \cdots & 0 & & x_{4,r} \\ \vdots & \vdots & \vdots & \ddots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 & & x_{r,r} \end{array}\right],$$

In a symbolic computational environment, as Mathematica®, we may find a family of GLMs of given order and IQS, depending on a set of free parameters. Then we may perform a numerical search for the method with maximal stability region. This is what it has been done in [5], [27], by suitably applying

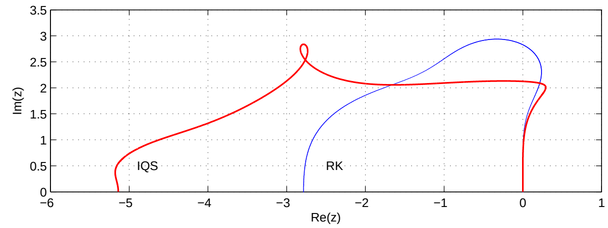

Fig. 1. Stability regions of RK method of order $p = 4$ and GLMs with $p = q = s = 4,\ r = 5$ with IQS

MATLAB functions like fminsearch. To obtain methods with larger stability regions, the IQS requirement can be relaxed, by asking for quadratic stability (QS), i.e. the stability polynomial has the form (17) [27], [28]. When the number of free parameters is large, as it happens for high order methods, the numerical search requires advanced optimization techniques, like those applied in [28].

Now we provide an example of method with IQS and maximal stability region. We set $p = q = s = 4$, $r = 5$. We fix vector $\mathbf{c}$ in advance. GLM method with the largest stability area has area equal to 18.3603, and error constant equal to -0.011. The stability polynomial is

$$p(w, z) = w^3(w^2 - p_4(z)w + p_3(z)),$$

with

$$\begin{aligned} p_4(z) &= 1 + \tfrac{293}{338}z + \tfrac{787}{1404}z^2 + \tfrac{1801}{9828}z^3 + \tfrac{265981}{12560184}z^4 \\ p_3(z) &= -\tfrac{45}{338}z - \tfrac{1325}{18252}z^2 + \tfrac{1349}{127764}z^3 + \tfrac{681937}{163282392}z^4. \end{aligned}$$

The method coefficients are

$$\mathbf{c} = [0, \frac{1}{3}, \frac{2}{3}, 1]^T, \tag{19}$$

$$\mathbf{A} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \end{bmatrix}, \tag{20}$$

$$\mathbf{V} = \begin{bmatrix} 1 & \frac{107}{169} & \frac{20}{117} & -\frac{1}{63} & -\frac{2}{71} \\ 0 & 0 & \frac{1}{2} & \frac{4}{27} & -\frac{7}{162} \\ 0 & 0 & 0 & \frac{1}{3} & \frac{5}{108} \\ 0 & 0 & 0 & 0 & \frac{1}{6} \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{21}$$

The other coefficient matrices can be derived from (14)-(16). In Fig. 1 we have plotted the stability region of this method and, for comparison, the stability region of explicit Runge–Kutta methods of order 4.

An efficient and accurate variable-step algorithm for solving non-stiff ODEs, based on explicit GLMs of Nordsieck type with QS or IQS must take into account fundamental issues, such as rescale strategy, local error estimation, step-changing strategy and starting procedure. Here we illustrate the technique that can be adopted. More details may be found in [6]. First we set

$$z^{[n]} = \begin{bmatrix} y_n \\ \overline{z}^{[n]} \end{bmatrix},$$

where $y_n \approx y(t_n)$ and $\overline{z}^{[n]} \approx z(t_n, h_n)$, $h_n = t_n - t_{n-1}$, with

$$z(t,h) := \begin{bmatrix} hy'(t) \\ h^2 y''(t) \\ \vdots \\ h^p y^{(p)}(t) \end{bmatrix}. \qquad (22)$$

Then GLM (2), on the nonuniform grid $t_0 < t_1 < \cdots < t_N, \quad t_N \geq T$, can be formulated as (compare [73])

$$\begin{cases} Y^{[n]} = (e \otimes I)y_{n-1} + h_n(A \otimes I)F(Y^{[n]}) \\ \qquad + (U \otimes I)z^{[n-1]}, \\ y_n = y_{n-1} + h_n(b^T \otimes I)F(Y^{[n]}) + (v^T \otimes I)z^{[n-1]}, \\ \overline{z}^{[n]} = h_n(B \otimes I)F(Y^{[n]}) + (V \otimes I)z^{[n-1]}, \end{cases} \qquad (23)$$

where

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} A & e & U \\ \hline b^T & 1 & v^T \\ B & 0 & V \end{array}\right], \qquad (24)$$

$e = [1, \ldots, 1]^T \in \mathbb{R}^s$, $b \in \mathbb{R}^s$, $v \in \mathbb{R}^{r-1}$, $A \in \mathbb{R}^{s \times s}$, $U \in \mathbb{R}^{s \times (r-1)}$, $B \in \mathbb{R}^{(r-1) \times s}$, $V \in \mathbb{R}^{(r-1) \times (r-1)}$.

The local error is analyzed by the following theorem [6] (compare also [15], [20], [73])

Theorem 2.7: Assume that the input quantities to the current step from t_{n-1} to $t_n = t_{n-1} + h_n$ satisfy

$$\begin{cases} y_{n-1} = y(t_{n-1}) \\ z^{[n-1]} = z(t_{n-1}, h_n) - (\beta \otimes I)h_n^{p+1} y^{(p+1)}(t_{n-1}) \\ \qquad + O(h_n^{p+2}) \end{cases} \qquad (25)$$

where $y(t)$ is the solution to the differential system (1) and require that

$$\begin{cases} y_n = y(t_n) - E h_n^{p+1} y^{(p+1)}(t_n) + O(h_n^{p+2}) \\ \overline{z}^{[n]} = \overline{z}(t_n, h_n) - (\beta \otimes I)h_n^{p+1} y^{(p+1)}(t_n) \\ \qquad + O(h_n^{p+2}) \end{cases} \qquad (26)$$

with the same vector β. Here, $\overline{z}(t_n, h_n)$ is the Nordsieck vector corresponding to the solution $\overline{y}(t)$ of the initial value problem

$$\begin{cases} \overline{y}'(t) = f(\overline{y}(t)), \qquad t \in [t_n, t_{n+1}], \\ \overline{y}(t_n) = y_n. \end{cases} \qquad (27)$$

Then it follows that (26) holds if

$$\begin{aligned} E &= \tfrac{1}{(p+1)!} - \tfrac{b^T c^p}{p!} + v^T \beta, \\ \beta &= (I - V)^{-1} \left(t_p - B \tfrac{c^p}{p!} \right), \\ t_p &= \begin{bmatrix} \tfrac{1}{p!} & \tfrac{1}{(p-1)!} & \cdots & 1 \end{bmatrix}^T. \end{aligned} \qquad (28)$$

According to the previous theorem, the local error is

$$le(t_n) = E h_n^{p+1} y^{(p+1)}(t_n) + O(h_n^{p+2}). \qquad (29)$$

The following result gives an estimate of the principal part of the local error, in the form

$$\begin{aligned} h_n^{p+1} y^{(p+1)}(t_n) = (\varphi^T \otimes \mathbf{I})h_n F(Y^{[n]}) \\ + (\psi^T \otimes \mathbf{I})z^{[n-1]} + O(h_n^{p+2}), \end{aligned} \qquad (30)$$

where $\mathbf{I}$ stands for the identity matrix of dimension d.

Theorem 2.8: Consider the GLM (23) of order p and stage order $q = p$ and assume that f is sufficiently smooth. The vectors $\varphi \in \mathbb{R}^s$ and $\psi \in \mathbb{R}^{r-1}$ in (60) satisfy the linear system

$$\begin{cases} \varphi^T \dfrac{\mathbf{c}^{j-1}}{(j-1)!} + \psi_j = 0, \quad j = 1, 2, \ldots, r-1, \\ \varphi^T \dfrac{\mathbf{c}^p}{p!} - \psi^T \beta = 1. \end{cases} \qquad (31)$$

Now we apply the previous theorem to the case $p = q = s = r - 1 = 4$, which covers the example of method (19)-(21). In such case, linear system (31) gives

$$\beta = \begin{bmatrix} \frac{1}{24} & \frac{1}{9} & \frac{29}{108} & \frac{1}{2} \end{bmatrix}^T, \quad E = \frac{26105531}{1632823920} \qquad (32)$$

$$\varphi = \begin{bmatrix} -429 & 486 & -243 & 54 \end{bmatrix}^T, \qquad (33)$$

$$\psi = \begin{bmatrix} 132 & -54 & 0 & 0 \end{bmatrix}^T. \qquad (34)$$

In a variable-step algorithm, a rescale strategy is also necessary when we have computed $\overline{z}^{[n]} \approx z(t_n, h_n)$ and should perform next step, since we need as a new input vector $z^{[n]} \approx z(t_n, h_{n+1})$, with $h_{n+1} = t_{n+1} - t_n$. A quite simple strategy to compute $z^[n]$ consists of rescaling the vector $z^{[n]}$, i.e.:

$$z^{[n]} = D(\delta)\overline{z}^{[n]}$$

with $D(\delta) = diag(\delta, \delta^2, \ldots, \delta^s)$, and $\delta = h_{n+1}/h_n$.
To complete the algorithm other ingredients are necessary, like an accurate starting procedure, a suitable choice of the initial step-size and step control strategy. Many different techniques can be applied, as illustrated in [6], [66], [67], [73].

For numerical comparison with other existing methods, we consider the linear test problem

$$y' = -\lambda y, \quad t \in [0, 10], \qquad (35)$$

for $\lambda = 50$ and the Prothero-Robinson type problem [78]

$$\begin{cases} y' = -16y + 15e^{-t}, \quad t \in [0, 100] \\ y(0) = 2 \end{cases} \qquad (36)$$

with exact solution $y(t) = e^{-t} + e^{-16t}$.
In Table I we list the error of Nordsieck method with IQS of order $p = 4$ (19)-(21) and of method with IRKS of the same order, corresponding to $\eta = 3/5$ with error constant $E = 1/300$, whose coefficients are given in [19]. We observe that the IQS method converges for a larger value of stepsize with respect to IRKS methods.

B. Implicit TSRK methods methods with quadratic stability

TSRK methods have the form

$$\begin{cases} Y_i^{[n]} = u_i y_{n-2} + (1 - u_i)y_{n-1} \\ \qquad + h \displaystyle\sum_{j=1}^{s} \Big(a_{ij} f(Y_j^{[n-1]}) + b_{ij} f(Y_j^{[n]}) \Big), \\ y_n = \theta y_{n-2} + (1 - \theta)y_{n-1} \\ \qquad + h \displaystyle\sum_{j=1}^{s} \Big(v_j f(Y_j^{[n-1]}) + w_j f(Y_j^{[n]}) \Big), \end{cases} \qquad (37)$$

TABLE I
ERRORS OF NORDSIECK METHOD AND IRKS METHOD OF ORDER $p = 4$ FOR PROBLEM (35), AND PROBLEM (36), WITH CONSTANT STEPSIZE.

problem (35), $\lambda = 50$			
N	h	IQS $p = 4$	IRKS $p = 4$
71	0.14	$8.33 \cdot 10^{+74}$	$1.75 \cdot 10^{+97}$
81	0.13	$5.59 \cdot 10^{+54}$	$4.42 \cdot 10^{+82}$
91	0.11	$3.70 \cdot 10^{+26}$	$1.28 \cdot 10^{+60}$
101	0.10	$2.92 \cdot 10^{-04}$	$3.48 \cdot 10^{+30}$
111	0.09	$2.83 \cdot 10^{-18}$	$2.97 \cdot 10^{-09}$
problem (36)			
N	h	IQS $p = 4$	IRKS $p = 4$
311	0.32	$1.02 \cdot 10^{+11}$	$1.06 \cdot 10^{+128}$
321	0.31	$3.68 \cdot 10^{-16}$	$2.85 \cdot 10^{+95}$
331	0.30	$1.02 \cdot 10^{-35}$	$8.50 \cdot 10^{+59}$
341	0.29	$1.08 \cdot 10^{-45}$	$1.08 \cdot 10^{+21}$
351	0.28	$4.14 \cdot 10^{-46}$	$1.47 \cdot 10^{-22}$

$i = 1, 2, \ldots, s$, $n = 2, 3, \ldots, N$, $Nh = T - t_0$. Here, y_n is an approximation of order p to $y(t_n)$, $t_n = t_0 + nh$, and $Y_i^{[n]}$ are approximations of stage order q to $y(t_{n-1} + c_i h)$, $i = 1, 2, \ldots, s$, where $y(t)$ is the solution to (1), $c = [c_1, \ldots, c_s]^T$ is the abscissa vector and $-1 < \theta \le 1$ for zero-stability.

Methods (37) can be reformulated as GLMs of the form

$$\left[\begin{array}{c} Y^{[n]} \\ \hline y_n \\ y_{n-1} \\ hf(Y^{[n]}) \end{array}\right] = \left[\begin{array}{c|ccc} B & e-u & u & A \\ \hline w^T & 1-\theta & \theta & v^T \\ 0 & 1 & 0 & 0 \\ I_s & 0 & 0 & 0 \end{array}\right] \left[\begin{array}{c} hf(Y^{[n]}) \\ \hline y_{n-1} \\ y_{n-2} \\ hf(Y^{[n-1]}) \end{array}\right]. \quad (38)$$

This representation corresponds to the problem (1) with $d = 1$ which is relevant in linear stability analysis. The matrices of the GLM (2) are then

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|ccc} B & e-u & u & A \\ \hline w^T & 1-\theta & \theta & v^T \\ 0 & 1 & 0 & 0 \\ I_s & 0 & 0 & 0 \end{array}\right] \in \mathbb{R}^{(2s+2)\times(2s+2)}, \quad (39)$$

In [35] the following theorem was proved, asserting that IQS condition leads to quadratic stability.

Theorem 2.9: Assume that the TSRK method (37) has IQS and that the matrices $I_s - z\mathbf{A}$ and $I_{s+2} - z\mathbf{X}$ are nonsingular. Then its stability function $p(\omega, z)$ defined by (5) assumes the form

$$p(\omega, z) = \omega^s\Big(\omega^2 - p_1(z)\omega + p_0(z)\Big), \quad (40)$$

where $p_1(z)$ and $p_0(z)$ are rational functions with respect to z.

In this section we will consider implicit methods where the matrix $\mathbf{A} = B$ has a one point spectrum, i.e.

$$\sigma(B) = \{\lambda\}, \quad \lambda > 0. \quad (41)$$

The feature of being one point spectrum would allow for efficient implementation of such methods similarly as in the case of singly implicit Runge-Kutta (SIRK) methods considered by Burrage [9], Butcher [12], and Burrage, Butcher and Chipman [10], see also [13], [15]. For methods for which the coefficient matrix B has a one point spectrum (41) it is more convenient to work with the function $\widetilde{p}(\omega, z)$ defined by

$$\widetilde{p}(\omega, z) = (1 - \lambda z)^s p(\omega, z), \quad (42)$$

in which the coefficients of ω^i, $i = 0, 1, \ldots, s+2$, are polynomials of degree s with respect to z. Then the if the IQS condition is verified the polynomial assumes the simple form

$$\widetilde{p}(\omega, z) = \omega^s\Big((1 - \lambda z)^s\omega^2 - \widetilde{p}_1(z)\omega + \widetilde{p}_0(z)\Big), \quad (43)$$

with a root $\omega = 0$ of multiplicity s, where $\widetilde{p}_1(z)$ and $\widetilde{p}_0(z)$ are polynomials of degree s with respect to z.

To express the IQS conditions (6) in terms of the coefficients θ, u, v, w, A, and B of TSRK method (37) we partition the matrix $\mathbf{X}$ as follows

$$\mathbf{X} = \left[\begin{array}{c|c} X_{11} & X_{12} \\ \hline X_{21} & X_{22} \end{array}\right], \quad (44)$$

where $X_{11} \in \mathbb{R}^{2\times 2}$, $X_{12} \in \mathbb{R}^{2\times s}$, $X_{21} \in \mathbb{R}^{s\times 2}$, $X_{22} \in \mathbb{R}^{s\times s}$. We also partition accordingly the matrices $\mathbf{B}$, $\mathbf{U}$, and $\mathbf{V}$ (see (39))

$$\mathbf{B} = \left[\begin{array}{c} B_{11} \\ \hline I_s \end{array}\right], \quad \mathbf{U} = \left[\begin{array}{c|c} U_{11} & A \end{array}\right], \quad \mathbf{V} = \left[\begin{array}{c|c} V_{11} & V_{12} \\ \hline 0 & 0 \end{array}\right],$$

where $B_{11} \in \mathbb{R}^{2\times s}$, $U_{11} \in \mathbb{R}^{s\times 2}$, $V_{11} \in \mathbb{R}^{2\times 2}$, $V_{12} \in \mathbb{R}^{2\times s}$ are given by

$$B_{11} = \begin{bmatrix} w^T \\ 0 \end{bmatrix}, \quad U_{11} = \begin{bmatrix} e-u & u \end{bmatrix},$$

$$V_{11} = \begin{bmatrix} 1-\theta & \theta \\ 1 & 0 \end{bmatrix}, \quad V_{12} = \begin{bmatrix} v^T \\ 0 \end{bmatrix},$$

and 0 in $\mathbf{V}$ stands for zero matrices of dimension $s \times 2$ and $s \times s$, respectively.

Theorem 2.10: A TSRK method (37) has IQS if there exist vectors $\alpha, \beta \in \mathbb{R}^s$ and a matrix $X \in \mathbb{R}^{s\times s}$ such that the following conditions are statisfied

$$B = \alpha w^T + X, \quad e = \alpha + \beta, \quad u = \theta\alpha, \quad A = \alpha v^T. \quad (45)$$

With the aim of constructing TSRK methods with IQS having order p and stage order $q = p$, we recall (see [35]) that, introducing the notation

$$C = \begin{bmatrix} c & \frac{c^2}{2!} & \cdots & \frac{c^s}{s!} \end{bmatrix}, \quad \widetilde{C} = \begin{bmatrix} e & \frac{c}{1!} & \cdots & \frac{c^{s-1}}{(s-1)!} \end{bmatrix},$$

$$d = \begin{bmatrix} -1 & \frac{1}{2!} & \cdots & \frac{(-1)^s}{s!} \end{bmatrix}^T, \quad g = \begin{bmatrix} 1 & \frac{1}{2!} & \cdots & \frac{1}{s!} \end{bmatrix}^T,$$

$$E = \begin{bmatrix} e & \frac{c-e}{1!} & \cdots & \frac{(c-e)^{s-1}}{(s-1)!} \end{bmatrix},$$

then the order p and stage order q conditions, with $q = p$, for TSRK method (37) take the form

$$AE = C - ud^T - B\widetilde{C}, \quad v^T E = g^T - \theta d^T - w^T\widetilde{C}. \quad (46)$$

Moreover the polynomials $\widetilde{p}_1(z)$ and $\widetilde{p}_2(z)$ appearing in (43) take the form

$$\widetilde{p}_1(z) = 1 - \theta + p_{11}z + \cdots + p_{1s}z^s,$$

$$\widetilde{p}_0(z) = -\theta + p_{01}z + \cdots + p_{0s}z^s.$$

Then the construction of highly stable TSRK methods (37) with IQS properties and coefficient matrix B with one point spectrum $\sigma(B) = \{\lambda\}$ can be summarized in the following algorithm.

1) Choose the abscissa vector c with distinct components, such that the matrices $\widetilde{C}$ and E defined at the beginning of this section are nonsingular.
2) As for methods of order $p = s$ the stability polynomial $\widetilde{p}(\omega, z)$ satisfies the condition
$$\widetilde{p}(e^z, z) = O(z^{s+1}), \quad z \to 0, \tag{47}$$
we solve this system by fixing s coefficients of the polynomials $\widetilde{p}_0(z)$ and $\widetilde{p}_1(z)$ and deriving the remaining s as functions of θ and λ. Choose the parameters θ and $\lambda > 0$ so that the stability polynomial $\widetilde{p}(\omega, z)$ is A-stable and also L-stable, by using the Schur criterion.
3) Compute the coefficient matrix B from the formula
$$B = (C - \alpha g^T)\widetilde{C}^{-1} + \alpha w^T,$$
which is a consequence of (46) and the last condition in (45). This matrix depends on the vectors α and w.
4) Compute the vectors β and u from the second and third condition of (45), i.e., $\beta = e - \alpha$ and $u = \theta\alpha$.
5) Compute the coefficient matrix A and the vector v from (46) as
$$A = (C - ud^T - B\widetilde{C})E^{-1}, \tag{48}$$
and
$$v^T = (g^T - \theta d^T - w^T\widetilde{C})E^{-1}. \tag{49}$$
They depend on α and w.
6) In order to impose that $\sigma(B) = \{\lambda\}$, solve the system
$$b_k(\theta, \alpha, c, w) = \begin{pmatrix} s \\ k \end{pmatrix}(-1)^k\lambda^k, \quad k = 1, 2, \ldots, s. \tag{50}$$
with respect to w, where $b_0 = 1$, and $b_k = b_k(\theta, \alpha, c, w)$, $k = 1, 2, \ldots, s$ are the coefficients of
$$\det(\omega I_s - B) = \sum_{k=0}^{s} b_k\omega^{s-k}.$$
This leads to a family of methods with IQS for which the matrix B has a one point spectrum $\sigma(B) = \{\lambda\}$.
7) Compute the matrix $\widetilde{M}_{11}(z)$ from the relation
$$\widetilde{M}_{11}(z) = M_{11}(z) + zM_{12}(z)(I_2 - zX)^{-1}[\ \alpha \quad \beta\ ], \tag{51}$$
where we $X = X_{22}$ in (44) and we have partitioned
$$\mathbf{M}(z) = \left[\begin{array}{c|c} M_{11}(z) & M_{12}(z) \\ \hline M_{21}(z) & M_{22}(z) \end{array}\right], \tag{52}$$
where $M_{11}(z) \in \mathbb{R}^{2\times 2}$, $M_{12}(z) \in \mathbb{R}^{2\times s}$, $M_{21}(z) \in \mathbb{R}^{s\times 2}$, $M_{22}(z) \in \mathbb{R}^{s\times s}$, and the stability polynomial $\widetilde{p}(\omega, z) = (1 - \lambda z)^s\omega^s \det(\omega I_2 - \widetilde{M}_{11}(z))$, whose coefficients p_{1j} and p_{0j} depend only on α.
8) Having computed the coefficients of the method in points 3, 4 and 5 such that the order conditions are satisfied up to order and stage order $p = q = s$, (47) is automatically satisfied by the polynomial $p(\omega, z)$ obtained in point 7. Then, in order to equate such stability polynomial with the one derived in point 2, it is sufficient to determine the parameter vector α by equalizing the s coefficients which have been fixed in point 2.

Now we provide an example of A- and L- stable TSRK method with $p = q = s = 4$. For $s = 4$ the stability polynomial (43) takes the form

$$\widetilde{p}(\omega, z) = \omega^4\Big((1 - \lambda z)^4\omega^2 - p_1(z)\omega + p_0(z)\Big),$$

with $p_1(z) = 1 - \theta + p_{11}z + p_{12}z^2 + p_{13}z^3$ and $p_0(z) = -\theta + p_{01}z + p_{02}z^2 + p_{03}z^3$. The system of equations corresponding to (47) with $s = 4$ takes the form

$$p_{11} - p_{01} = 1 - 4\lambda + \theta, \quad 2p_{11} + 2p_{12} - 2p_{02} = 3 - 16\lambda + 12\lambda^2 + \theta,$$

$$3p_{11} + 6p_{12} + 6p_{13} - 6p_{03} = 7 - 48\lambda + 72\lambda^2 - 24\lambda^3 + \theta,$$

$$4p_{11} + 12p_{12} + 24p_{13} = 15 - 128\lambda + 288\lambda^2 - 192\lambda^3 + 24\lambda^4 + \theta,$$

and assuming that $p_{13} = 0$ and $p_{03} = 0$ the unique solution to this system is given by

$$p_{11} = \frac{1 - 32\lambda + 144\lambda^2 - 144\lambda^3 + 24\lambda^4 - \theta}{2},$$

$$p_{12} = \frac{17 - 192\lambda + 576\lambda^2 - 480\lambda^3 + 72\lambda^4 - \theta}{12},$$

$$p_{01} = \frac{3 - 40\lambda + 144\lambda^2 - 144\lambda^3 + 24\lambda^4 + \theta}{2},$$

$$p_{02} = \frac{7 - 96\lambda + 360\lambda^2 - 384\lambda^3 + 72\lambda^4 + \theta}{12}.$$

The range of parameters (θ, λ) for which the $p(\omega, z)$ is A-stable and also L-stable is plotted in Fig. 2 by the shaded region. The regions were obtained by computer searches in the parameter space (θ, λ) using the Schur criterion [79], [76].

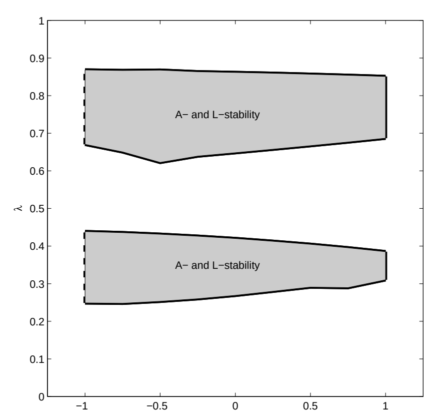

Fig. 2. Regions of A-stability and L-stability in the (θ, λ)-plane for $p(\omega, z)$ with $p = s = 4$.

The coefficients of the method corresponding to $\lambda = \frac{1}{3}$ and the abscissa vector $c = [0, \frac{1}{3}, \frac{2}{3}, 1]^T$ are given by

$$A = \begin{bmatrix} -\frac{73571}{418565} & \frac{316790}{450193} & -\frac{383309}{370547} & -\frac{1102057}{1459404} \\ -\frac{324116}{495273} & \frac{3108022}{1186313} & -\frac{2008351}{521461} & -\frac{1905671}{677809} \\ -\frac{813738}{787901} & \frac{4021146}{972541} & -\frac{6409321}{1054477} & -\frac{6349415}{1430988} \\ -\frac{426460}{370257} & \frac{4154204}{900915} & -\frac{12185608}{1797671} & -\frac{6621076}{1338039} \end{bmatrix},$$

$$B = \begin{bmatrix} \frac{1082275}{789096} & -\frac{47158}{1102905} & -\frac{20658}{230377} & \frac{16548}{733283} \\ \frac{2053468}{392523} & \frac{173881}{1660851} & -\frac{337517}{836884} & \frac{86197}{880374} \\ \frac{13765224}{1684843} & \frac{119918}{620675} & -\frac{387828}{932779} & \frac{214966}{1621163} \\ \frac{8694859}{954168} & \frac{68987}{727614} & -\frac{198815}{935168} & \frac{90358}{331129} \end{bmatrix},$$

$$v = \begin{bmatrix} -\frac{426460}{370257} & \frac{4154204}{900915} & -\frac{12185608}{1797671} & -\frac{6621076}{1338039} \end{bmatrix}^T,$$

$$w = \begin{bmatrix} \frac{8694859}{954168} & \frac{68987}{727614} & -\frac{198815}{935168} & \frac{90358}{331129} \end{bmatrix}^T.$$

The stability polynomial $p(\omega, z)$ of this method is

$$p(\omega, z) = \omega^4\Big(\Big(1 - \frac{1}{3}z\Big)^4\omega^2 - p_1(z)\omega + p_0(z)\Big)$$

with

$$p_1(z) = 1 - \frac{744347}{1148421}z + \frac{2965}{320219}z^2,$$
$$p_0(z) = -\frac{241021}{765596}z - \frac{198226}{1427227}z^2.$$

In order to demonstrate that the TSRK methods of order p and stage order $q = p$ do not suffer from order reduction which is the case for classical Runge-Kutta formulas, we have applied the Runge-Kutta-Gauss method of order $p = 4$ and stage order $q = 2$ and TSRK method of order $p = 4$ and stage order $q = 4$ givenabove to the van der Pol oscillator (see VDPOL problem in [67])

$$\begin{cases} y_1' = y_2, & y_1(0) = 2, \\ y_2' = \big((1 - y_1^2)y_2 - y_1\big)/\epsilon, & y_2(0) = -2/3, \end{cases} \tag{53}$$

$t \in [0, T]$, with a stiffness parameter ϵ.

The results of numerical experiments for fixed stepsize implementations of Runge-Kutta-Gauss method of order $p = 4$ and stage order $q = 2$ and TSRK method of order $p = 4$ and stage order $q = 4$ are presented in Table II-B. These results correspond to $T = 2/3$, $h = T/N$, and $N = 32$, 64, 128, 256 and 512. In these tables we have listed norms of errors $\|e_h^{RKG}(T)\|$ and $\|e_h^{TSRK}(T)\|$ at the endpoint of integration T and the observed order of convergence p computed from the formula

$$p = \frac{\log\big(\|e_h(T)\|/\|e_{h/2}(T)\|\big)}{\log(2)},$$

where $e_h(T)$ and $e_{h/2}(T)$ are errors corresponding to stepsizes h and $h/2$ for Runge-Kutta-Gauss and TSRK methods.

We can observe that for small values of ϵ ($\epsilon = 10^{-6}$) for which the van der Pol oscillator (53) is stiff the Runge-Kutta Gauss method exhibits order reduction phenomenon and its order of convergence drops to about $p = 2$ which corresponds

	$\epsilon = 10^{-6}$		$\epsilon = 10^{-6}$	
N	$\|e_h^{TSRK}(T)\|$	p	$\|e_h^{TSRK}(T)\|$	p
32	$5.83 \cdot 10^{-3}$		$2.44 \cdot 10^{-4}$	
64	$1.49 \cdot 10^{-3}$	1.97	$2.65 \cdot 10^{-5}$	3.21
128	$3.71 \cdot 10^{-4}$	2.01	$2.20 \cdot 10^{-6}$	3.59
256	$8.84 \cdot 10^{-5}$	2.07	$1.59 \cdot 10^{-7}$	3.79
512	$1.87 \cdot 10^{-5}$	2.24	$1.08 \cdot 10^{-8}$	3.89

TABLE II
COMPARISON BETWEEN RKG METHOD OF ORDER $p = 4$ AND STAGE ORDER $q = 2$ AND TSRK METHOD OF ORDER $p = 4$ AND STAGE ORDER $q = 4$

to the stage order $q = 2$. This is not the case for TSRK method which preserves order of convergence $p = q = 4$, which leads to higher accuracy.

III. ALGEBRAIC STABILITY

Consider the nonlinear test problem nonlinear test problem

$$\begin{cases} y'(t) = g\big(t, y(t)\big), & t \geq 0, \\ y(0) = y_0, \end{cases} \tag{54}$$

$g : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$. Here, the function g satisfies the one-sided Lipschitz condition of the form

$$\big(g(t, y_1) - g(t, y_2)\big)^T(y_1 - y_2) \leq 0, \tag{55}$$

for all $t \geq 0$ and $y_1, y_2 \in \mathbb{R}^d$. Denote by $y(t)$ and $\widetilde{y}(t)$ two solutions to (54) with initial conditions y_0 and $\widetilde{y}_0$, respectively. Then the condition (55) implies that (54) is dissipative, i.e.,

$$\big\|y(t_2) - \widetilde{y}(t_2)\big\| \leq \big\|y(t_1) - \widetilde{y}(t_1)\big\|, \tag{56}$$

for $0 \leq t_1 \leq t_2$, compare [16], [73].

Definition 3.1: Let $\{z^{[n]}\}_{n=0}^N$ be the solution to (2) with initial value $z^{[0]}$, and by $\{\widetilde{z}^{[n]}\}_{n=0}^N$ be the solution obtained by using a different initial value $\widetilde{z}^{[0]}$ or by perturbing the right hand side of (54). A GLM (2) is said to be G-stable if there exists a real, symmetric and positive definite matrix $\mathbf{G} \in \mathbb{R}^{r\times r}$ such that

$$\big\|z^{[n+1]} - \widetilde{z}^{[n+1]}\big\|_G \leq \big\|z^{[n]} - \widetilde{z}^{[n]}\big\|_G, \tag{57}$$

for all step sizes $h > 0$ and for all differential systems (54) with the function g satisfying (55), where

$$\|z\|_G^2 = \sum_{i=1}^r\sum_{j=1}^r g_{ij}z_i^Tz_j, \qquad z_i \in \mathbb{R}^d,\ i = 1, 2, \ldots, r. \tag{58}$$

Observe that the notion of G-stability is not only useful in order to give a nice characterization of methods able to preserve the contractivity of solutions of dissipative problems, but also to give a complete characterization of numerical methods retaining the same invariants of conservative problems, such as Hamiltonian problems: this issue has given rise to the notion of G-symplecticity (see [15], [17], [48], [49], [54], [55] and references therein).

We now aim to give a characterization of G-stability which only requires the fulfillment of simple algebraic constraints in place of (57), which is certainly hard to prove in general. To do this, we provide the following definition.

Definition 3.2: The GLM (2) 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 $\mathbf{D} \in \mathbb{R}^{m\times m}$ such that the matrix $\mathbf{M} \in \mathbb{R}^{(m+r)\times(m+r)}$ defined by

$$\mathbf{M} = \left[\begin{array}{c|c} \mathbf{DA} + \mathbf{A}^T\mathbf{D} - \mathbf{B}^T\mathbf{GB} & \mathbf{DU} - \mathbf{B}^T\mathbf{GV} \\ \hline \mathbf{U}^T\mathbf{D} - \mathbf{V}^T\mathbf{GB} & \mathbf{G} - \mathbf{V}^T\mathbf{GV} \end{array}\right] \quad (59)$$

is nonnegative definite.

The significance of this definition follows from the result proved by Butcher [14], that for preconsistent and non-confluent GLMs (2), i.e. methods with distinct abscissas c_i, $i = 1, 2, \ldots, m$, algebraic stability is equivalent to G-stability.

It was observed by Hewitt and Hill [68], [69] that the verification if the matrix $\mathbf{M}$ is nonnegative definite can be simplified by the use of the following result proved by Albert [1].

Theorem 3.1: (Albert Theorem) 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

$$\begin{array}{l} \mathbf{M}_{11} \geq 0, \quad \mathbf{M}_{22} - \mathbf{M}_{12}^T\mathbf{M}_{11}^+\mathbf{M}_{12} \geq 0, \\ \mathbf{M}_{11}\mathbf{M}_{11}^+\mathbf{M}_{12} = \mathbf{M}_{12}, \end{array} \quad (60)$$

or, equivalently,

$$\begin{array}{l} \mathbf{M}_{22} \geq 0, \quad \mathbf{M}_{11} - \mathbf{M}_{12}\mathbf{M}_{22}^+\mathbf{M}_{12}^T \geq 0, \\ \mathbf{M}_{22}\mathbf{M}_{22}^+\mathbf{M}_{12}^T = \mathbf{M}_{12}^T. \end{array} \quad (61)$$

Here, $\mathbf{A}^+$ stands for the Moore-Penrose pseudo-inverse of the matrix $\mathbf{A}$.

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. In fact, in [37], [69] the authors propose a simplified version of conditions (61), considering $\mathbf{G} = I$ and with some simplifications in order to find algebraically stable TSRK methods whose coefficients are expressed in rational form.

In [36], instead, an optimization-based numerical approach has been used to derive the coefficients of algebraically stable TSRK methods and two-step almost collocation (TSAC) methods, respectively. 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 introduced in [72], to which we refer for more details. The above mentioned approach is based on the Nyquist stability function, defined by

$$\mathbf{N}(\xi) = \mathbf{A} + \mathbf{U}(\xi\mathbf{I} - \mathbf{V})^{-1}\mathbf{B}, \quad \xi \in \mathbb{C} \setminus \sigma(\mathbf{V}), \quad (62)$$

where $\sigma(\mathbf{V})$ stands for the spectrum of the matrix $\mathbf{V}$. A detailed explanation on the derivation of the Nyquist function in the general setting of GLMs, together with its connections with control theory, can be found in [70], Section 5. Following [70], we denote by $\widetilde{\mathbf{w}}$ a principal left eigenvector of $\mathbf{V}$, i.e. the vector such that

$$\widetilde{\mathbf{w}}^T\mathbf{V} = \widetilde{\mathbf{w}}^T, \quad \widetilde{\mathbf{w}}^T\mathbf{q}_0 = 1, \quad (63)$$

where $\mathbf{q}_0$ is the preconsistency vector of GLMs. We next define the diagonal matrix $\widetilde{\mathbf{D}}$ by

$$\widetilde{\mathbf{D}} = \mathrm{diag}(\mathbf{B}^T\widetilde{\mathbf{w}}), \quad (64)$$

and by $\mathrm{He}(\mathbf{Q})$ the Hermitian part of a complex square matrix $\mathbf{Q}$, i.e.,

$$\mathrm{He}(\mathbf{Q}) = \frac{1}{2}\big(\mathbf{Q} + \mathbf{Q}^*\big),$$

where $\mathbf{Q}^*$ stands for the conjugate transpose of $\mathbf{Q}$. We have the following result.

Theorem 3.2: (compare [14], [70]). A consistent GLM (2) is algebraically stable if the following conditions are satisfied:

1) the coefficient matrix $\mathbf{V}$ is power-bounded;
2) $\mathbf{Ux} \neq \mathbf{0}$ for all right eigenvectors of $\mathbf{V}$ and $\mathbf{B}^T\mathbf{x} \neq \mathbf{0}$ for all left eigenvectors of $\mathbf{V}$;
3) $\widetilde{\mathbf{D}} > 0$ and $\widetilde{\mathbf{D}}\mathbf{A} \geq 0$;
4) $\mathrm{He}\big(\widetilde{\mathbf{D}}\mathbf{N}(\xi)\big) \geq 0$ for all ξ such that $|\xi| = 1$ and $\xi \in \mathbb{C} \setminus \sigma(\mathbf{V})$.

We now describe the construction of algebraically stable TSRK methods belonging to the subclass of TSAC methods [51]. TSAC methods are continous methods of the form:

$$\begin{cases} P(t_n + sh) = \varphi_0(s)y_{n-1} + \varphi_1(s)y_n \\ \quad + h\displaystyle\sum_{j=1}^{m}\Big(\chi_j(s)f(P(t_{n-1} + c_jh)) + \psi_j(s)f(P(t_n + c_jh))\Big), \\ y_{n+1} = P(t_{n+1}), \end{cases} \quad (65)$$

where $t_n = t_0 + nh$, $n = 0, 1, \ldots, N$, $Nh = T - t_0$, is a uniform grid. The continuous approximant $P(t_n + sh)$ is an algebraic polynomial which can be expressed as linear combination of the basis functions

$$\{\varphi_0(s),\ \varphi_1(s),\ \chi_j(s),\ \psi_j(s),\ j = 1, 2, \ldots, m\},$$

which are unknown algebraic polynomials to be suitably determined.

We observe that by evaluating the collocation polynomial at $s = 1$ and $s = c_i$, $i = 1, 2, \ldots, m$, and by setting $Y_i^{[n]} = P(t_n + c_ih)$, $i = 1, 2, \ldots, m$, TSAC methods (37) can be formulated as TSRK methods

$$\begin{cases} y_{n+1} = \theta y_{n-1} + \widetilde{\theta}y_n \\ \qquad + h\displaystyle\sum_{i=1}^{m}\Big(v_if(Y_i^{[n]}) + w_if(Y_i^{[n-1]})\Big), \\ Y_i^{[n]} = u_iy_{n-1} + \widetilde{u}_iy_n \\ \qquad + h\displaystyle\sum_{j=1}^{m}\Big(a_{ij}f(Y_j^{[n]}) + b_{ij}f(Y_j^{[n-1]})\Big), \end{cases} \quad (66)$$

where

$$\theta = \varphi_0(1), \quad \widetilde{\theta} = \varphi_1(1), \quad v_i = \psi_i(1), \quad w_i = \chi_i(1),$$
$$u_i = \varphi_0(c_i), \quad \widetilde{u}_i = \varphi_1(c_i), \quad a_{ij} = \psi_j(c_i), \quad b_{ij} = \chi_j(c_i),$$

$i,j=1,2,\ldots,m$. Observe that $\widetilde{\theta}=1-\theta$ and $\widetilde{u}_i=1-u_i,\ i=1,2,\ldots,m$

It is generally required that the polynomial $P(t_n+sh)$ in (65) satisfies the interpolation conditions

$$P(t_{n-1})=y_{n-1},\quad P(t_n)=y_n, \tag{67}$$

and the collocation conditions

$$\begin{aligned} P'(t_{n-1}+c_jh)&=f(P(t_{n-1}+c_jh)),\\ P'(t_n+c_jh)&=f(P(t_n+c_jh)), \end{aligned} \tag{68}$$

$j=1,2,\ldots,m$. However, in order to obtain methods with strong stability properties such as, for example, A- or L-stability, we relax some of the interpolation and collocation conditions. This leads to additional free parameters which are then used to obtain methods with desirable stability properties. Following the terminology introduced in [51] the resulting methods are called TSAC methods.

Such methods are obtained by fixing ρ basis functions among the set

$$\{\varphi_0(s),\ \chi_j(s),\ j=1,2,\ldots,m\}, \tag{69}$$

as polynomials of degree $p=2m+1-\rho$, and deriving the remaining ones as solutions of the system of order conditions

$$\begin{cases} \varphi_0(s)+\varphi_1(s)=1,\\ \dfrac{(-1)^k}{k!}\varphi_0(s)+\\ +\displaystyle\sum_{j=1}^m\left(\chi_j(s)\frac{(c_j-1)^{k-1}}{(k-1)!}+\psi_j(s)\frac{c_j^{k-1}}{(k-1)!}\right)=\frac{s^k}{k!}, \end{cases} \tag{70}$$

$k=1,2,\ldots,p$. Then, it was proved in [51], that $p=2m+1-\rho$ is the uniform order of the resulting method.

In the paper [36] an algorithm was developed for the numerical search of TSAC methods written as GLMs (2). This algorithm is based on minimizing the objective function which computes the negative value of the minimum of the eigenvalues of the matrix

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi)),\quad \text{for } \xi \text{ such that } |\xi|=1 \text{ and } \xi\in\mathbb{C}\setminus\sigma(\mathbf{V}). \tag{71}$$

Such matrix has been computed in [36] for TSAC methods and assumes the form

$$\begin{aligned}\mathrm{He}\big(\widetilde{\mathbf{D}}\mathbf{N}(\xi)\big)=\frac{1}{2(1+\theta)}\Bigg(&\mathrm{diag}(v+w)\Big(A+\frac{1}{\xi}B\Big)\\ &+\Big(A^T+\frac{1}{\bar{\xi}}B^T\Big)\mathrm{diag}(v+w)\\ &+\Big(\frac{\xi}{(\xi-1)(\xi+\theta)}+\frac{\bar{\xi}}{(\bar{\xi}-1)(\bar{\xi}+\theta)}\Big)vv^T\\ &+\Big(\frac{1}{(\xi-1)(\xi+\theta)}+\frac{\bar{\xi}}{(\bar{\xi}-1)(\bar{\xi}+\theta)}\Big)vw^T\\ &+\Big(\frac{\xi}{(\xi-1)(\xi+\theta)}+\frac{1}{(\bar{\xi}-1)(\bar{\xi}+\theta)}\Big)wv^T\\ &+\Big(\frac{1}{(\xi-1)(\xi+\theta)}+\frac{1}{(\bar{\xi}-1)(\bar{\xi}+\theta)}\Big)ww^T\\ &-\frac{1}{\xi+\theta}\big((v+w)\cdot u\big)v^T-\frac{1}{\bar{\xi}+\theta}v\big((v+w)\cdot u\big)^T\\ &-\frac{1}{\xi(\xi+\theta)}\big((v+w)\cdot u\big)w^T-\frac{1}{\bar{\xi}(\bar{\xi}+\theta)}w\big((v+w)\cdot u\big)^T\Bigg).\end{aligned}$$

Once order conditions are imposed and the other desired properties are achieved, the matrix (71) will depend on a certain number P of free parameters $a_1,a_2,\ldots,a_P$. Such parameters will be chosen in order to satisfy condition 4 of Theorem 3.2, i.e.

$$\mathrm{He}\big(\widetilde{\mathbf{D}}\mathbf{N}(\xi)\big)\Big|_{\xi=e^{it}}\geq 0,\quad t\in[0,2\pi], \tag{72}$$

by means of the objective function

$$f(a_1,a_2,\ldots,a_P)=-\min_{j,k}\lambda_{jk}(a_1,a_2,\ldots,a_P),$$

which is a numerical realization of the mentioned necessary condition, where $\{\lambda_{jk}(a_1,a_2,\ldots,a_P):k=1,2,\ldots,m\}$ is the spectrum of the matrix $\mathrm{He}\big(\widetilde{\mathbf{D}}\mathbf{N}(e^{i\frac{2\pi}{n}j})\big)$, $j=1,2,\ldots,n-1$, $n\in\mathbb{N}$, being i the imaginary unit. We observe that we did not consider the values $j=0$ and $j=n$ because they lead to points belonging to the spectrum of the matrix $\mathbf{V}$. By increasing the number n of points on the unit circle we search for methods satisfying (72), and the remaining necessary conditions 1-3 in Theorem 3.2 for algebraic stability are verified on the case by case basis.

Since A-stable TSAC methods with $m=1,2,3$ and $p>m+1$ have not been found in previous works (compare [51]), the search of algebraically stable methods has been performed among TSAC methods of order $p=m$ or $p=m+1$.

We now provide and example of method with $m=2$ and $p=3$. We carry out the search inside the class of A-stable methods derived in [51]. Therefore, following [51], we impose the interpolation conditions

$$\varphi_0(0)=0,\quad \chi_1(0)=0,$$

and we fix the $\rho=2$ basis functions

$$\varphi_0(s)=s\left(q_2s^2+q_1s+q_0\right),\quad \chi_1(s)=s\left(r_2s^2+r_1s+r_0\right),$$

where q_2, q_1, q_0, r_2, r_1, and r_0 are real parameters. We next derive the values of these parameters realizing the collocation conditions

$$\varphi_0'(c_1) = \varphi_0'(c_2) = 0 \quad \text{and} \quad \chi_1'(c_1) = \chi_1'(c_2) = 0.$$

This leads to

$$q_1 = -\frac{(c_1+c_2)q_0}{2c_1c_2}, \quad q_2 = \frac{q_0}{3c_1c_2},$$
$$r_1 = -\frac{(c_1+c_2)r_0}{2c_1c_2}, \quad r_2 = \frac{r_0}{3c_1c_2}.$$

We next determine the remaining basis functions $\varphi_1(s)$, $\chi_2(s)$, $\psi_1(s)$, and $\psi_2(s)$ by imposing the system of order conditions for $p = 3$. As in [51], we fix $c_1 = 5/2$ and $c_2 = 9/2$. This leads to a two-parameter family of TSAC methods, depending on q_0 and r_0. Within this family, we search for algebraically stable methods, by minimizing the negative value of the objective function computing the minimum of the eigenvalues of the matrix (71). For instance, for

$$q_0 = -0.4253608181543406, \quad r_0 = 1.6033382155047602, \tag{73}$$

we obtain a method satisfying

$$\mathrm{He}(\widetilde{\mathbf{D}}\mathbf{N}(\xi))\Big|_{\xi=e^{it}} \geq 0, \quad t \in [0, 2\pi].$$

This bound has been obtained by dividing the interval $[0, 2\pi]$ into $n = 10000$ subintervals.

IV. Conclusions

We described the construction of highly stable explicit and implicit GLMs. Namely, by using the IQS approach, we described the construction of explicit GLMs of Nordsiek type having maximum area of the stability region, and A- and L-stablle implicit TSRK methods. We moreover presebnted the approaches for the systematic search for algebraically stable GLMs for ODEs, based on the Albert theorem and the criteria formulated by Hill, which are based on the Nyquist stability function. In all cases we presented example of methods. Further issues of this research will focus on analyzing nonlinear stability issues of numerical methods approximating other functional operators such as integral and fractional equations [11], [21], [25], [33], [42], partial differential equations [26], [29]–[31], [39], [58], [61], oscillatory problems [40], [43], [59], [62], [65], [77].

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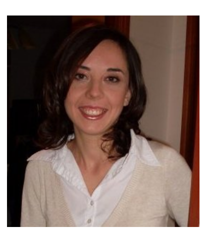

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