P-stable General Nyström methods for $y'' = f(y(t))$

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Abstract

We focus our attention on the family of General Linear Methods (GLMs), for the numerical solution of second order ordinary differential equations (ODEs). These are multivalue methods introduced in [18] with the aim to provide an unifying approach for the analysis of the properties of accuracy of numerical methods for second order ODEs. Our investigation is addressed to providing the building blocks useful to analyze the linear stability properties of GLMs for second order ODEs: thus, we present the extension of the classical notions of stability matrix, stability polynomial, stability and periodicity interval, A-stability and P-stability to the family of GLMs. Special attention will be given to the derivation of highly stable GLMs, whose stability properties depend on the stability polynomial of indirect Runge-Kutta-Nyström methods based on Gauss-Legendre collocation points, which are known to be P-stable. In this way, we are able to provide P-stable GLMs whose order of convergence is greater than that of the corresponding RKN method, without heightening the computational cost. We finally provide and discuss examples of P-stable irreducible GLMs satisfying the mentioned features.

Key words: Second order Ordinary Differential Equations, General Linear Methods, Linear stability analysis, P-stability.

1. Introduction

The paper is focused on the numerical solution of initial value problems based on special second order ODEs

$$\begin{cases} y''(t) = f(y(t)), & t \in [t_0, T], \\ y(t_0) = y_0, \\ y'(t_0) = y'_0, \end{cases} \tag{1.1}$$

being the function $f : \mathbb{R}^d \to \mathbb{R}^d$ smooth enough in order to guarantee the Hadamard well-posedness of the problem. Even though the problem (1.1) might be regarded as an equivalent doubled dimensional system of first order ODEs, the direct solution of the second order version results to be more natural and efficient [23, 25].

We frame our treatise in the context of General Linear methods for second order ODEs (1.1), introduced by the authors in [18] and here denoted as General Linear

Nyström (GLN) methods. In this paper we assume the following formulation for the family of GLN methods

$$\begin{aligned} Y_i^{[n]} &= h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} y_j^{[n-1]}, \quad i = 1, ..., s, \\ y_i^{[n]} &= h^2 \sum_{j=1}^{s} b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} y_j^{[n-1]}, \quad i = 1, ..., r, \end{aligned} \tag{1.2}$$

where the vector

$$y^{[n-1]} = \begin{bmatrix} y_1^{[n-1]} \\ y_2^{[n-1]} \\ \vdots \\ y_r^{[n-1]} \end{bmatrix} \in \mathbb{R}^{rd},$$

denoted as *input vector* of the external stages contains all the informations we transfer from point t_{n-1} to point t_n of the grid. We observe that such vector might also not only contain approximations to the solution of the problem in the grid points inherited from previous steps, but also other informations computed in the past that we aim to use in the integration process.

The vector

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ Y_2^{[n]} \\ \vdots \\ Y_s^{[n]} \end{bmatrix} \in \mathbb{R}^{sd},$$

is instead denoted as vector of the *internal* stages and its entries provide approximations to the solution in the internal points $t_{n-1} + c_j h,\ j = 1, 2, \ldots, s$.

GLN methods (1.2) can also be represented in terms of the coefficient matrices $\mathbf{A} \in \mathbb{R}^{\mathbf{s}\times\mathbf{s}}$, $\mathbf{U} \in \mathbb{R}^{\mathbf{s}\times\mathbf{r}}$, $\mathbf{B} \in \mathbb{R}^{\mathbf{r}\times\mathbf{s}}$, $\mathbf{V} \in \mathbb{R}^{\mathbf{r}\times\mathbf{r}}$, which are put together in the following partitioned $(s + r) \times (s + r)$ matrix

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right]. \tag{1.3}$$

Using these notations, a GLM for second order ODEs admits the following tensor representation

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A} \otimes \mathbf{I})F^{[n]} + (\mathbf{U} \otimes \mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B} \otimes \mathbf{I})F^{[n]} + (\mathbf{V} \otimes \mathbf{I})y^{[n-1]}, \end{aligned} \tag{1.4}$$

where $\otimes$ denotes the usual Kronecker tensor product, $\mathbf{I}$ is the identity matrix in $\mathbb{R}^{d\times d}$ and $F^{[n]} = [f(Y_1^{[n]})^T,\ f(Y_2^{[n]})^T,\ \ldots,\ f(Y_s^{[n]})^T]^T$.

We observe that the formulation introduced in [18], i.e.

$$
\begin{aligned}
Y^{[n]} &= h^2(\mathbf{A}\otimes\mathbf{I})F^{[n]} + h(\mathbf{P}\otimes\mathbf{I})y'^{[n-1]} + (\mathbf{U}\otimes\mathbf{I})y^{[n-1]},\\
hy'^{[n]} &= h^2(\mathbf{C}\otimes\mathbf{I})F^{[n]} + h(\mathbf{R}\otimes\mathbf{I})y'^{[n-1]} + (\mathbf{W}\otimes\mathbf{I})y^{[n-1]},\\
y^{[n]} &= h^2(\mathbf{B}\otimes\mathbf{I})F^{[n]} + h(\mathbf{Q}\otimes\mathbf{I})y'^{[n-1]} + (\mathbf{V}\otimes\mathbf{I})y^{[n-1]},
\end{aligned}
\tag{1.5}
$$

differs from (1.4), where the first derivative approximations are not emphasized as in (1.5). In the *hybrid* formulation (1.4) employed here

- the first derivative approximations might be hidden in the vector $y^{[n]}$ of the external stages as it happens, for instance, when it approximates the Nordsieck vector (compare, for instance, [26] and the references therein)

$$
z_n = \begin{bmatrix} y(t_n) \\ hy'(t_n) \\ \vdots \\ h^{r-1}y^{(r-1)}(t_n) \end{bmatrix};
\tag{1.6}
$$

- approximations of the first derivative might be completely neglected in the numerical integration process, as it is the case of hybrid methods (compare, for instance, [7, 14, 15, 16, 17] and references therein).

The specific scope of this paper is the derivation of high order P-stable GLN methods which result to be competitive with classical P-stable methods known in the literature, such as Runge-Kutta-Nyström methods based on indirect collocation on Gauss-Legendre points. In order to succeed in pursuing this goal, rather than neglecting such known highly stable methods, we aim to let GLN formulae inherit their stability polynomial through imposing simple algebraic constraints on the coefficients of the methods: this property will be denoted in the remainder of the paper as *Runge-Kutta-Nyström stability*. In this way, some coefficients of the GLN will be constrained to reproduce the stability properties of a reference Runge-Kutta-Nyström (RKN) method, while the remaining degrees of freedom will be employed to achieve a certain order of convergence, possibly heightening that of the reference RKN method.

The paper is organized as follows: Section 2 is devoted to the convergence analysis of GLN methods (1.2), by suitably applying the results formerly presented in [18]; Section 3 regards the linear stability analysis of GLN methods (1.2), with the particular aim to the provide the extension of the classical notions of stability matrix, stability polynomial, stability and periodicity intervals, A-stability and P-stability to the family of GLN methods; Section 4 introduces the notion of RKN-stability for the family of GLN methods. We aim to find examples of GLN formulae with RKN-stability of higher order than that of the reference RKN method: the derivation of such examples will be carried out within the family of Nordsieck GLN methods, which is introduced and analyzed in Section 5. RKN-stability reveals to be a practical way to derive high order P-stable methods: examples oriented in this direction are reported in Section 6, where the derived methods are also compared with classical P-stable RKN method on a famous periodic stiff problem. Some conclusions are object of Section 7.

2. Convergence analysis

In this section, we suitably extend to the class of GLN methods (1.2) the basic concepts of consistency, zero-stability and convergence introduced in [18] for the general formulation (1.5). These properties provide the minimal requirements of accuracy and stability for the numerical solution of ODEs, as well known in the literature (compare, for instance, the monographs [1, 2, 23, 26]).

Minimal accuracy requests for numerical methods solving (1.1) are achieved if the components of the input and output vectors $y^{[n-1]}$ and $y^{[n]}$ in (1.4) respectively satisfy (compare [18])

$$y_i^{[n-1]} = q_{i,0}y(t_{n-1}) + q_{i,1}hy'(t_{n-1}) + q_{i,2}h^2y''(t_{n-1}) + O(h^3),$$

$$y_i^{[n]} = q_{i,0}y(t_n) + q_{i,1}hy'(t_n) + q_{i,2}h^2y''(t_n) + O(h^3),$$

$i = 1, 2, \ldots, r$. We also assume that the components of the stage vector $Y^{[n]}$ in (1.4) fulfill the condition

$$Y_i^{[n]} = y(t_{n-1} + c_i h) + O(h^3), \quad i = 1, \ldots, s.$$

The above minimal accuracy demandings are achieved if a GLN method (1.4) satisfies the algebraic constraints on the coefficient matrices introduced in the following definitions, which are the adaptations to the hybrid case (1.4) of the concepts introduced in [18].

Definition 2.1. *A GLM (1.2) is preconsistent if there exist two vectors* $\mathbf{q}_0$ *and* $\mathbf{q}_1$ *such that*

$$\mathbf{U}\mathbf{q}_0 = e, \quad \mathbf{V}\mathbf{q}_0 = \mathbf{q}_0, \quad \mathbf{U}\mathbf{q}_1 = \mathbf{c}, \quad \mathbf{V}\mathbf{q}_1 = \mathbf{q}_0 + \mathbf{q}_1, \tag{2.1}$$

where $\mathbf{c}$ *denotes the abscissa vector of the method.*

Definition 2.2. *A preconsistent GLM (1.2) is consistent if there exists a vector* $\mathbf{q}_2$ *such that*

$$\mathbf{B}e + \mathbf{V}\mathbf{q}_2 = \frac{\mathbf{q}_0}{2} + \mathbf{q}_1 + \mathbf{q}_2. \tag{2.2}$$

Definition 2.3. *A consistent GLM (1.2) is stage-consistent if*

$$\mathbf{A}e + \mathbf{U}\mathbf{q}_2 = \frac{\mathbf{c}^2}{2}.$$

The minimal stability demanding are instead achieved by applying the GLM (1.4) to the problem

$$y'' = 0,$$

obtaining the recurrence relation

$$y^{[n]} = \mathbf{V}y^{[n-1]},$$

which leads to the following definition.

Definition 2.4. *A GLN (1.4) is zero-stable if there exist two real constants C and D such that*

$$\|\mathbf{V}^m\| \leq mC + D, \quad \forall m = 1, 2, \ldots. \tag{2.3}$$

This definition assures that the classical root condition for numerical methods solving second order ODEs (1.2) is satisfied. Such a condition is reported in point (*ii*) of the following theorem (compare [18]).

Theorem 2.1.
The following statements are equivalent:

(i) the matrix $\mathbf{V}$ *satisfies the bound (2.3);*
(ii) the roots of the minimal polynomial of the matrix $\mathbf{V}$ *lie on or within the unit circle and the multiplicity of the zeros on the unit circle is at most two;*
(iii) there exists a matrix B similar to $\mathbf{V}$ *such that*

$$\sup_{m\geq 1} \|B^m\|_\infty \leq m + 1.$$

We remark that condition (*ii*) in Theorem 2.1 is peculiar for numerical methods for second order ODEs (1.1), because for classical methods for first order ODEs at most one root of the zero-stability matrix is allowed to have modulus one. Here two roots of the minimal polynomial of the zero-stability might lie on the unit circle, also recovering the case of complex conjugate roots of modulus one, typical of the oscillatory case (compare [23]).

We finally introduce a suitable notion of convergence, by adapting that introduced in [18]. In force of the multivalue nature of GLN methods (1.4), a starting procedure is needed in order to determine the missing starting vector $y^{[0]}$: in the context of convergence analysis, we only need to assume that there exist a starting procedure

$$S_h : \mathbb{R}^d \to \mathbb{R}^{dr},$$

associating, for any value of the stepsize h, a starting vector $y^{[0]} = S_h(y_0)$ such that

$$\lim_{h\to 0} \frac{S_h(y_0) - (\mathbf{q_0} \otimes I)y(t_0)}{h} = (\mathbf{q_1} \otimes I)y'(t_0). \tag{2.4}$$

The following definition is correspondingly given.

Definition 2.5. *A preconsistent GLN method (1.2) is convergent if, for any well-posed initial value problem (1.1), there exist a starting procedure S_h satisfying (2.4) such that the sequence of vectors $y^{[n]}$, computed using n steps with stepsize $h = (\bar{t} - t_0)/n$ and using $y^{[0]} = S_h(y_0)$, converges to $\mathbf{q}_0 y(\bar{t})$, for any $\bar{t} \in [t_0, T]$.*

As usual in the numerical integration of ODEs, consistency and zero-stability are the needed ingredients producing the convergence of the method. From [18], the following theorem holds.

Theorem 2.2. *A GLN method* (1.2) *is convergent if and only if it is consistent and zero-stable.*

3. Linear stability analysis

We now focus our attention to the analysis of the linear stability properties of GLN methods (1.2). Linear stability demandings for numerical methods solving second order ODEs (1.1) are classically provided with respect to the scalar linear test equation

$$y'' = -\lambda^2 y, \tag{3.1}$$

introduced by Lambert and Watson in [28]. Applying the GLN method in tensor form (1.4) to the test equation (3.1), we obtain

$$Y^{[n]} = -\lambda^2 h^2 \mathbf{A} Y^{[n]} + \mathbf{U} y^{[n-1]}, \tag{3.2}$$

$$y^{[n]} = -\lambda^2 h^2 \mathbf{B} Y^{[n]} + \mathbf{V} y^{[n-1]}. \tag{3.3}$$

We set $z = \lambda h$ and $\Lambda = (\mathbf{I} + z^2\mathbf{A})^{-1}$, assuming that the matrix $\mathbf{I} + z^2\mathbf{A}$ is invertible. Then it follows from (3.2) that

$$Y^{[n]} = \Lambda \mathbf{U} y^{[n-1]},$$

and substituting this relation for the internal stages into (3.3), we obtain

$$y^{[n]} = \mathbf{M}(z^2) y^{[n-1]},$$

where the matrix $\mathbf{M}(z^2)$, defined by

$$\mathbf{M}(z^2) = \mathbf{V} - z^2 \mathbf{B} \Lambda \mathbf{U} \in \mathbb{R}^{r\times r},$$

is the so-called *stability* (or *amplification*) matrix, while its characteristic polynomial $p(\omega, z^2)$ is denoted as *stability polynomial*. This is a polynomial of degree r with respect to ω and its coefficients are rational functions with respect to z^2.

We now introduce the following definitions extending the classical notions of periodicity interval and P-stability to the family of GLN methods (1.2) [29, 32].

Definition 3.1. $(0, H_0^2)$ *is a periodicity interval for the method (1.2) if,* $\forall z^2 \in (0, H_0^2)$, *the stability polynomial* $p(\omega, z^2)$ *has two complex conjugate roots of modulus 1, while all the others have modulus less than 1.*

Definition 3.2. *A GLM is $P-$ stable if its periodicity interval is* $(0, +\infty)$.

The importance of P-stability lies in its ability to efficiently integrate *periodic stiff* problems as clarified, for instance, in [31]. Such problems are characterized by a periodic theoretical solution expressed as combination of components with dominant short frequencies and components with large frequencies and small amplitudes. An accurate numerical solution of periodic stiff problems would impose severe restriction on the stepsize length. However, this limit can be efficiently overcome by applying P-stable methods, since P-stability ensures that the choice of the stepsize is independent from the values of the frequencies, but it only depends on the desired accuracy [9, 30, 31]. In some sense, this notion completely parallels that of A-stability for first order ODEs, since A-stable methods are particularly relevant in the numerical solution of stiff problems, eliminating any stepsize restriction due to stability reasons (compare, for instance, [2, 24] and references therein).

4. Runge-Kutta-Nyström stability

In [28], the authors proved that P-stable linear multistep methods for second order ODEs (1.1)

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j f(t_{n+j}, y_{n+j}).$$

can achieve maximum order 2. Moreover, Coleman [8] proved that no P-stable one step symmetric collocation methods exist.

In the context of RKN methods [24, 29]

$$\begin{aligned}
Y_i &= y_n + c_i h y'_n + h^2 \sum_{j=1}^{s} a_{ij} f(t_n + c_j h, Y_j), \quad i = 1, 2, ..., s, \\
y_{n+1} &= y_n + h y'_n + h^2 \sum_{i=1}^{s} \bar{b}_i f(t_n + c_i h, Y_i), \\
y'_{n+1} &= y'_n + h \sum_{i=1}^{s} b_i f(t_n + c_i h, Y_i),
\end{aligned}$$

many A-stable and P-stable methods exist, but the ones falling in the subclass of direct collocation methods, whose coefficients (see [23]) have the form

$$\begin{aligned}
a_{ij} &= \int_0^{c_i} L_j(s) ds, \\
b_i &= \int_0^{1} L_i(s) ds, \\
\bar{b}_i &= \int_0^{1} (1 - s) L_i(s) ds,
\end{aligned}$$

have only bounded stability intervals and are not P-stable [30].

In the context of collocation methods for second order equations, interesting insights in the possibility of achieving a good balance between order of convergence and P-stability come from the family of so-called *indirect* collocation formulae [10, 32]. Indirect collocation methods are generated by applying a collocation based Runge-Kutta method (for the classical idea of numerical collocation and its extensions compare [2, 12, 13, 19, 20, 22, 23]) to the first order representation of (1.1). Given a (c, A, b) collocation based Runge-Kutta method, the tableau of the corresponding indirect collocation method is

$$\begin{array}{c|c}
c & A^2 \\
\hline
 & A^T b \\
 & b^T
\end{array}$$

which results in a Runge-Kutta-Nyström method [23]. The theory of indirect collocation methods completely parallels the well–known theory of collocation methods for first order equations (see [32]) and, therefore, the properties of a collocation method are totally inherited by the corresponding indirect collocation method. Thus, the maximum attainable order is $2s$, where s is the number of stages, and it is achieved by Gauss-type methods, which are also A-stable, while L-stability is achieved by Radau IIA-type methods, of order $2s-1$.

It is important to highlight the fact that indirect collocation methods based on the Gauss-Legendre collocation points are P-stable (compare [32]). Such methods have order $2s$ and stage order s and represent, at the best of our knowledge, the family of P-stable methods with the highest order of convergence with respect to those known in the literature. This is the starting point in our search for high order P-stable GLN methods (1.2), compare [21]. In order to understand this aspect, let us make a digression to the first order case.

In the context of the numerical integration of first order ODEs, Runge-Kutta methods provide an excellent balance between strong stability properties and high order of convergence. For this reason, in recent times, the attention of many authors has been devoted to the construction of GLMs for first order ODEs having the same stability properties of Runge-Kutta methods (see [2, 26] and references therein). Thus, if $\mathbf{M}(z) \in \mathbb{R}^{r\times r}$ is the stability matrix of a certain GLM, this method is said to be *Runge-Kutta stable* if its stability polynomial $p(\omega, z)$ takes the form

$$p(\omega, z) = \omega^{r-1}(\omega - R(z)),$$

where $R(z)$ is the stability function of a reference Runge-Kutta method. This means that the corresponding GLM inherits the same stability properties of the Runge-Kutta method assumed as reference. Butcher and Wright (see [2, 4, 26] and references therein) characterized Runge-Kutta stability in terms of algebraic conditions on the coefficient matrices of the method, introducing the concept of *inherent Runge-Kutta stability*.

Following the above described lines drawn in the literature in the context of GLMs for first order ODEs (also compare [3, 5, 6, 11]), we introduce an analogous notion of stability for GLN methods (1.2), in order to let these methods inherit the same stability properties of a certain RKN method assumed as reference.

Definition 4.1. *A GLN method* (1.2) *is said to be* ***Runge-Kutta-Nyström stable*** *if its stability polynomial assumes the form*

$$p(\omega, z^2) = \omega^{r-2}\left(q_2(z)\omega^2 + q_1(z)\omega + q_0(z)\right),$$

where $q_2(z)\omega^2 + q_1(z)\omega + q_0(z)$ *is the stability polynomial of a certain reference Runge-Kutta-Nyström method.*

In other words, the stability properties of GLN methods methods having RKN-stability are determined by the polynomial

$$q_2(z)\omega^2 + q_1(z)\omega + q_0(z),$$

which is exactly the stability polynomial of a RKN method. Therefore GLN methods (1.2) with RKN-stability on Gaussian points are A-stable and, in particular, P-stable.

Section 6 reports examples of GLN methods with RKN-stability which result to be P-stable and having higher order of convergence than that of the corresponding reference RKN method, i.e., that based on indirect collocation on Gaussian points. Such examples are derived within the family of GLN methods (1.2) whose input vector approximates the so-called Nordsieck vector. This family of methods is introduced in next section.

5. GLN methods of Nordsieck type

We now assume that the input vector $y^{[n]}$ of the GLN (1.2) approximates the so-called Nordsieck vector (compare [26] and references therein)

$$\begin{bmatrix} y(t_n) \\ hy'(t_n) \\ \vdots \\ h^p y^p(t_n) \end{bmatrix}, \tag{5.1}$$

i.e. the i-th entry $y_i^{[n]}$ of the input vector approximates the scaled i-th derivative $h^i y^{(i-1)}(t_n)$, $i = 0, 1, \ldots, p$, where p is the order of convergence of the method. We observe that, since the input vector and the Nordsieck one respectively have dimensions r and $p+1$, we will always assume that $r = p + 1$.

As a direct consequence of the form of the input vector, the vectors $\mathbf{q}_0$, $\mathbf{q}_1$ and $\mathbf{q}_2$ involved in the definitions of preconsistency and consistency, have the form

$$\mathbf{q}_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \mathbf{q}_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \mathbf{q}_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}.$$

Hence, for a Nordsieck GLN, the vectors $\mathbf{q}_0$, $\mathbf{q}_1$ and $\mathbf{q}_2$ are the first three vectors e_1, e_2, e_3 in the canonical basis of R^r. This remark is helpful in order to provide a complete convergence analysis of GLN methods in Nordsieck form, which is given in the following result.

Theorem 5.1. *A GLN* (1.4) *whose input vector $y^{[n]}$ approximates the Nordsieck vector* (5.1) *is convergent if and only if*

(*i*) $\mathbf{B}e + \mathbf{V}\mathbf{q}_2 = \dfrac{e_1}{2} + e_2 + e_3$;

(*ii*) *its Butcher tableau has the form*

$$\left[\begin{array}{c|ccc} \mathbf{A} & e & c & \widetilde{U} \\ \hline \mathbf{B} & e_1 & e_1 + e_2 & \widetilde{V} \end{array}\right],$$

where $\widetilde{U} \in \mathbb{R}^{s\times(r-2)}$ and $\widetilde{V} \in \mathbb{R}^{s\times(r-2)}$;

(*iii*) *all the eigenvalues of* $\overline{V}$ *have modulus strictly less than 1, being* $\overline{V}$ *the matrix* $\widetilde{V}$ *deprived of its first two rows.*

Proof: In force of the criterion provided by Theorem 2.2, we are allowed to establish the analysis of convergence of GLN methods (1.4) on proving preconsistency, consistency and zero-stability. Since in the case of Nordsieck methods the vectors $\mathbf{q}_0$ and $\mathbf{q}_1$ are the first two vectors e_1, e_2 of the canonical basis in $\mathbb{R}^r$, the conditions of preconsistency (2.1) applied to such methods assume the form

$$\mathbf{U}e_1 = e, \quad \mathbf{V}e_1 = e_1, \quad \mathbf{U}e_2 = \mathbf{c}, \quad \mathbf{V}e_2 = e_1 + e_2,$$

providing that the first two columns of the matrix $\mathbf{U}$ are the vectors e and $\mathbf{c}$, respectively, while those of the matrix $\mathbf{V}$ are e_1 and $e_1 + e_2$, respectively, which gives the point (*ii*) of the thesis.

Point (*i*) of the thesis is, instead, direct consequence of consistency condition (2.2), where the vectors $\mathbf{q}_0$, $\mathbf{q}_1$ and $\mathbf{q}_2$ are replaced by e_1, e_2 and e_3, respectively. Once consistency is assessed, the remaining point to analyze is zero-stability. Thus, we investigate if the root condition (*ii*) in Theorem 2.1 is satisfied. This point is clarified by observing the expression of the matrix $\mathbf{V}$ once preconsistency is imposed, which assumes the following form

$$\mathbf{V} = \left[\begin{array}{cc|c} 1 & 0 & \widetilde{v}_1 \\ 1 & 1 & \widetilde{v}_2 \\ \hline 0 & 0 & \\ \vdots & \vdots & \overline{V} \\ 0 & 0 & \end{array}\right],$$

where $\widetilde{v}_1$ and $\widetilde{v}_2$ are the first two rows of the matrix $\widetilde{V}$. Hence, the matrix $\mathbf{V}$ of a preconsistent GLN in Nordsieck form is block lower triangular. As a consequence, the root condition (*ii*) in Theorem 2.1, which guarantees the zero-stability of the method, is satisfied if the eigenvalues of $\overline{V}$ are all in modulus strictly less than 1. This implies point (*iii*) of the thesis and completes the proof. □

Theorem 5.1 suggests that the first two columns of the matrices $\mathbf{U}$ and $\mathbf{V}$ play a special role in the convergence of a GLN method (1.2) in Nordsieck form. We now prove that the remaining columns of $\mathbf{U}$ and $\mathbf{V}$ dictate the order of convergence of the method.

Theorem 5.2. *A GLN method* (1.4) *in Nordsieck form has order and stage-order both equal to p if and only if*

$$\begin{aligned} v^{(k+1)} &= \sum_{\ell=0}^{k} \frac{e_{k-\ell+1}}{\ell!} - \frac{\mathbf{B}\mathbf{c}^{k-2}}{(k-2)!}, \\ u^{(k+1)} &= \frac{\mathbf{c}^k}{k!} - \frac{\mathbf{A}\mathbf{c}^{k-2}}{(k-2)!}, \end{aligned} \tag{5.2}$$

$k = 2, \ldots, p+1$, *being* $v^{(k+1)}$ *and* $u^{(k+1)}$ *the* $(k+1)$*-st columns of the matrices* $\mathbf{U}$ *and* $\mathbf{V}$*, respectively.*

Proof: We remind (compare [18]) that a GLN has order p if and only if, by definition,

$$y_i^{[n]} = \sum_{j=0}^{p} q_{j,i} h^j y^j(t_n) + O(h^{p+1}).$$

Correspondingly, it is known from the general theory of GLN methods (compare [18]) that such a method has order and stage-order p if and only if

$$\begin{aligned} &\mathbf{c}^k - k(k-1)\mathbf{A}\mathbf{c}^{k-2} - k!\mathbf{U}\mathbf{q}_k = 0, \\ &\sum_{\ell=0}^{k} \frac{k!}{\ell!}\mathbf{q}_{k-\ell} - k(k-1)\mathbf{B}\mathbf{c}^{k-2} - k!\mathbf{V}\mathbf{q}_k = 0, \end{aligned}$$

for $k = 2\ldots, p+1$. In the case of GLN methods in Nordsieck form, the vectors $\mathbf{q}_j$, $j = 0, 1, \ldots, p$ form the canonical basis of $\mathbb{R}^r$ since $r = p+1$. Thus, the above system of order conditions assume the form

$$\begin{aligned} &\mathbf{c}^k - k(k-1)\mathbf{A}\mathbf{c}^{k-2} - k!\mathbf{U}e_{k+1} = 0, \\ &\sum_{l=0}^{k} \frac{k!}{l!} e_{k-l+1} - k(k-1)\mathbf{B}\mathbf{c}^{k-2} - k!\mathbf{V}e_{k+1} = 0, \end{aligned}$$

for $k = 2\ldots, p+1$, which is equivalent to (5.2), completing the proof. □

We observe that order conditions (5.2) also holds true when the order p and stage-order q differs by one, i.e. when $q = p-1$ (compare [18, 26]).

6. Derivation of P-stable methods

We now apply all the tools introduced in the previous sections to derive examples of RKN-stable GLN methods (1.4) whose input vector approximates the Nordsieck vector (5.1). In particular, as first examples, we suppose that the dimension of the internal stage vector is $s = 1$ and assume as reference RKN method the one based on indirect collocation on one Gauss-Legendre point

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{4} \\ \hline & \frac{1}{2} \\ & 1 \end{array} \tag{6.1}$$

whose stability polynomial is

$$q(\omega, z^2) = \omega^2 + \frac{2\left(-4+z^2\right)}{4+z^2}\omega + 1,$$

thus it is P-stable.

In order to make a comparison among formulae having the same computational cost, since method (6.1) has order 2, we look for one-stage GLN methods (thus, having the same computational cost of (6.1)) of order greater than 2. Hence, in our derivation process:

- we impose the conditions guaranteeing the convergence of the method, given in Theorem 5.1;
- we derive the remaining columns of the matrices **U** and **V** given by Theorem 5.1, in order to achieve order of convergence at least equal to 3;
- we force the remaining degrees of freedom to provide a stability polynomial of the form
$$p(\omega, z^2) = \omega^{r-2}\left(\omega^2 + \frac{2\left(-4+z^2\right)}{4+z^2}\omega + 1\right),$$
ensuring that the corresponding method is automatically P-stable.

Since $r = p+1$ and we wish order at least equal to 3, we first assume $r = 4$. We correspondingly obtain a one-stage P-stable method of order $p = 3$ and stage order $q = 2$, with $c = \frac{2-\sqrt{2}}{2}$ and

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cccc} \frac{1}{4} & 1 & \frac{2-\sqrt{2}}{2} & \frac{1-\sqrt{2}}{2} & \frac{1-\sqrt{2}}{6} \\ \hline \frac{3+2\sqrt{2}}{6} & 1 & 1 & -\frac{\sqrt{2}}{3} & -\frac{\sqrt{2}}{12} \\ \frac{5+3\sqrt{2}}{6} & 0 & 1 & \frac{1-3\sqrt{2}}{6} & \frac{2-\sqrt{2}}{12} \\ \frac{2+\sqrt{2}}{2} & 0 & 0 & -\frac{\sqrt{2}}{2} & \frac{1}{2} \\ 1 & 0 & 0 & -1 & \frac{\sqrt{2}}{2} \end{array}\right].$$

If $r = 5$, we gain a one-stage P-stable method of order $p = 4$ and stage order $q = 3$, with $\mathbf{A} = \left[\frac{1}{4}\right]$,

$$\mathbf{U} = \left[\begin{array}{ccccc} 1 & c & \frac{-1+2c^2}{4} & \frac{1}{12}\left(\frac{3c}{2}+c^3\right) & \frac{c\left(-3+c^3\right)}{24} \end{array}\right],$$

$$\mathbf{B} = \left[\begin{array}{c} \frac{42-64c+37c^2-10c^3+c^4}{24} \\ \frac{67-76c+30c^2-4c^3}{24} \\ \frac{(-3+c)(-2+c)}{2} \\ \frac{5}{2}-c \\ 1 \end{array}\right],$$

$$
\mathbf{V} = \begin{bmatrix} 1 & 1 & \frac{-30+64c-37c^2+10c^3-c^4}{24} & \frac{4-42c+64c^2-37c^3+10c^4-c^5}{24} & \frac{2-42c^2+64c^3-37c^4+10c^5-c^6}{48} \\ 0 & 1 & \frac{-43+76c-30c^2+4c^3}{24} & \frac{12-67c+76c^2-30c^3+4c^4}{24} & \frac{16-67c^2+76c^3-30c^4+4c^5}{48} \\ 0 & 0 & \frac{-4+5c-c^2}{2} & \frac{2-6c+5c^2-c^3}{2} & \frac{2-6c^2+5c^3-c^4}{4} \\ 0 & 0 & c-\frac{5}{2} & 1-\frac{5c}{2}+c^2 & \frac{4-5c^2+2c^3}{4} \\ 0 & 0 & -1 & -c & 1-\frac{c^2}{2} \end{bmatrix},
$$

where $c \approx 0.3754243604533405$ is the only root in $(0, 1)$ of the polynomial

$$
a(x) = 6 - 210x^3 + 320x^4 - 185x^5 + 50x^6 - 5x^7,
$$

having two pairs of complex conjugate roots and two real roots outside the interval $(0, 1)$.

This order 4 method (denoted as GLN4) is now compared with the RKN one considered as reference method, i.e. the indirect collocation RKN method based on one Gauss-Legendre collocation point (next denoted as RKN2). They are both one-stage methods, thus they require the same computational cost for the integration process. Such methods are applied on the periodic stiff problem introduced by Kramarz in [27]

$$
y''(t) = \begin{bmatrix} \mu-2 & 2\mu-2 \\ 1-\mu & 1-2\mu \end{bmatrix} y(t), \quad t \in [0, 20\pi]
$$

with initial conditions

$$
y(0) = [2, -1]^T, \quad y'(0) = [0, 0]^T.
$$

The eigenvalues of the Jacobian of the coefficient matrix of the problem are -1, $-\mu$: consequently, the analytical solution of the system depends on the two frequencies 1 and $\sqrt{\mu}$. However, the high frequency component, corresponding to $\sqrt{\mu}$ when $\mu \gg 1$, is eliminated by the initial conditions: the exact solution is indeed $y(t) = [2\cos(t), -\cos(t)]^T$. Notwithstanding this, its presence in the general solution of the system dictates restrictions on the choice of the stepsize, so that the system is stiff.

We show the numerical evidence originated by applying the two methods in a fixed stepsize environment, with stepsize

$$
h = \frac{\pi}{2^k},
$$

being k an integer number. The results, reported in Table 1, experimentally confirm the theoretical order of convergence and reveal the superiority of the GLN4 method.

7. Conclusions

We have analyzed the stability properties of GLN methods (1.4) and investigated the possibility of obtaining P-stable formulae of higher order than that known in the

k	RKN2			GLN4		
	$\|\|err(20\pi)\|\|_\infty$	p	fe	$\|\|err(20\pi)\|\|_\infty$	p	fe
3	$4.47 \cdot 10^{-1}$		477	$5.86 \cdot 10^{-1}$		480
4	$1.24 \cdot 10^{-1}$	1.98	957	$3.99 \cdot 10^{-2}$	3.87	959
5	$2.82 \cdot 10^{-2}$	1.99	1917	$2.53 \cdot 10^{-3}$	3.98	1916
6	$7.05 \cdot 10^{-3}$	1.99	3837	$1.59 \cdot 10^{-4}$	3.99	3838
7	$1.76 \cdot 10^{-3}$	2.00	7677	$9.94 \cdot 10^{-6}$	4.00	7670
8	$4.41 \cdot 10^{-4}$	2.00	15357	$6.21 \cdot 10^{-7}$	4.00	15340

Table 1: Numerical results for RKN2 and GLN4 on Kramarz problem, where $err(20\pi)$ is the global error in the endpoint of the integration, p is estimated order of convergence, fe the number of function evaluations

literature, without heightening the computational cost. To succeed in this aim we have first selected a family of reference P-stable methods, namely the class RKN method based on indirect collocation on Gauss-Legendre points, and forced our methods to inherit the same stability polynomial. This leads to the concept of RKN-stability. We have introduced RKN-stable GLN methods (1.4) whose input vector is the Nordsieck vector (5.1). As first examples, we have derived P-stable methods of order 3 and 4 of convergence, which is higher than that of the analog RKN reference method, without heightening the computational cost. The numerical evidence confirm the theoretical order of convergence and confirm the effectiveness and efficiency of the introduced methods. The introduced technique can be next used to develop methods depending on a larger number of internal stages, which result to have order of convergence higher than that of the reference RKN method.

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