Multivalue approximation of second order differential problems: a review

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Abstract—We present a collection of recent results on the numerical approximation of second order differential problems of the type $y'' = f(y(t))$ by means of family of multivalue numerical methods, here denoted as generalized Nyström methods. These methods can be thought as a general family of formulae for the numerical approximation of second order problems, which properly include classical formulae, such as linear multistep methods and Runge-Kutta-Nyström methods, but also enable to find new methods which provide better balances between accuracy and stability demandings. This is made possible because generalized Nyström methods rely on a larger number of degrees of freedom than classical methods, which can be employed for the mentioned purposes. We provide the formulation of the family of methods, showing that existing methods can be regarded according to the new formalism, study the main properties and give examples of highly stable genuine multivalue methods whose order is higher than that of existing methods. In particular, we aim to inherit the best stability properties known in the literature, i.e. those coming from Gauss-Legendre points leading to P-stable methods, by introducing generalized Nyström methods having with the same stability polynomial of Gauss-Legendre methods but higher order of convergence. We show that it is possible to obtain P-stable methods with order 4 relying on one single internal stage (in the classical case, the maximum attainable order is only 2, requiring the same computational cost). A numerical experiment shows the effectiveness of the approach on a periodic stiff problem, also in comparison with existing methods.

Keywords—Multivalue numerical methods, general linear methods, second order problems, P-stability

I. Formalism of multivalue methods

Our investigation is here focused on the numerical approximation of initial value problems based on special second order ordinary differential equations (ODEs)

$$\begin{cases} y''(t) = f(y(t)), \quad t \in [t_0, T], \\ y(t_0) = y_0 \in \mathbb{R}^d, \\ y'(t_0) = y'_0 \in \mathbb{R}^d, \end{cases} \tag{1}$$

where the function $f : \mathbb{R}^d \to \mathbb{R}^d$ is smooth enough to ensure the Hadamard well-posedness of the differential problem. Though problem (1) admits the equivalent first order formulation, the consequent augmentation of the dimensionality makes the direct integration of the second order problem favourable.

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In [44], a general framework for the numerical approximation of (1) has been introduced (also compare [40], [43], [52], [54]; see [3], [6], [22], [64] and references therein for the first order case) in order to assess an unifying strategy for the analysis of accuracy and stability requirements to be asked for, such as consistency, zero-stability and convergence, when developing acceptable numerical methods. Such a general family is of multivalue type, i.e. the approximation of a set of r solution related and r' derivative related values is provided and inherited from a step point to the following one, generalizing an approach of Runge-Kutta type. To be more detailes, let us recall the formulation of these methods which be called, from now on, *generalized Nyström methods* (GNMs). To this purpose, in correspondence of the fixed stepsize discretization

$$t_0 \leq t_1 \leq \cdots \leq T_N = T,$$

of the interval $[t_0, T]$, we define the following supervectors

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

$$y'^{[n-1]} = \begin{bmatrix} y'^{[n-1]}_1 \\ y'^{[n-1]}_2 \\ \vdots \\ y'^{[n-1]}_{r'} \end{bmatrix} \in \mathbb{R}^{r'd},$$

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

The vector $y^{[n-1]}$, denoted as *input vector* of the external stages, approximates the r solution related values transferred from the point t_{n-1} to t_n of the discretization. Analogously, the vector $y'^{[n-1]}$ contains the r' derivative related values computed in t_{n-1}, while the values $Y_j^{[n-1]}$, denoted as *internal stage* values, provide an approximation to the solution in the internal points $t_{n-1} + c_j h$, $j = 1, 2, \ldots, s$.

We next introduce the following coefficient matrices $\mathbf{A} \in \mathbb{R}^{\mathbf{s}\times\mathbf{s}}$, $\mathbf{P} \in \mathbb{R}^{\mathbf{s}\times\mathbf{r}'}$, $\mathbf{U} \in \mathbb{R}^{\mathbf{s}\times\mathbf{r}}$, $\mathbf{C} \in \mathbb{R}^{\mathbf{r}'\times\mathbf{s}}$, $\mathbf{R} \in \mathbb{R}^{\mathbf{r}'\times\mathbf{r}'}$, $\mathbf{W} \in \mathbb{R}^{\mathbf{r}'\times\mathbf{r}}$, $\mathbf{B} \in \mathbb{R}^{\mathbf{r}\times\mathbf{s}}$, $\mathbf{Q} \in \mathbb{R}^{\mathbf{r}\times\mathbf{r}'}$, $\mathbf{V} \in \mathbb{R}^{\mathbf{r}\times\mathbf{r}}$, collected in the following partitioned $(s+r'+r)\times(s+r'+r)$ matrix

$$\left[\begin{array}{c|c|c} \mathbf{A} & \mathbf{P} & \mathbf{U} \\ \hline \mathbf{C} & \mathbf{R} & \mathbf{W} \\ \hline \mathbf{B} & \mathbf{Q} & \mathbf{V} \end{array}\right], \tag{2}$$

which is the Butcher tableau of GNMs. Correspondingly, GNMs are formulated as follows

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A}\otimes\mathbf{I})F^{[n]} + h(\mathbf{P}\otimes\mathbf{I})y'^{[n-1]} \\ &\quad + (\mathbf{U}\otimes\mathbf{I})y^{[n-1]}, \\ hy'^{[n]} &= h^2(\mathbf{C}\otimes\mathbf{I})F^{[n]} + h(\mathbf{R}\otimes\mathbf{I})y'^{[n-1]} \\ &\quad + (\mathbf{W}\otimes\mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B}\otimes\mathbf{I})F^{[n]} + h(\mathbf{Q}\otimes\mathbf{I})y'^{[n-1]} \\ &\quad + (\mathbf{V}\otimes\mathbf{I})y^{[n-1]}, \end{aligned} \tag{3}$$

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

In absence of dependence on $y'^{[n-1]}$, the matrices $\mathbf{P}, \mathbf{Q}, \mathbf{C}, \mathbf{R}, \mathbf{W}$ do not contribute to the multivalue numerical dynamics and, in such a case, the reduced tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right], \tag{4}$$

completely characterizes GNMs, which will correspondingly have the *hybrid* formulation

$$\begin{aligned} Y^{[n]} &= h^2(\mathbf{A}\otimes\mathbf{I})F^{[n]} + (\mathbf{U}\otimes\mathbf{I})y^{[n-1]}, \\ y^{[n]} &= h^2(\mathbf{B}\otimes\mathbf{I})F^{[n]} + (\mathbf{V}\otimes\mathbf{I})y^{[n-1]}. \end{aligned} \tag{5}$$

A. Classical methods recasted as GNMs

The family of GNMs properly contains, as special cases, many numerical methods for (1) already introduced in the existing literature, as clarified by the following examples.

1) Linear multistep methods. Linear multistep methods for second order ODEs [57], [59], defined by

$$y_n = \sum_{j=1}^{k} \alpha_j y_{n-j} + h^2 \sum_{j=0}^{k} \beta_j f(y_{n-j}), \tag{6}$$

can be regarded as GNMs with $r=2k$, $s=1$, $Y^{[n]}=[y_n]$,

$$y^{[n-1]} = \begin{bmatrix} y_{n-1} \\ y_{n-2} \\ \vdots \\ y_{n-k} \\ h^2 f(y_{n-1}) \\ h^2 f(y_{n-2}) \\ \vdots \\ h^2 f(y_{n-k}) \end{bmatrix},$$

and in correspondence to the reduced tableau (4)

$$\left[\begin{array}{c|cccccccc} \beta_0 & \alpha_1 & \ldots & \alpha_{k-1} & \alpha_k & \beta_1 & \ldots & \beta_{k-1} & \beta_k \\ \hline \beta_0 & \alpha_1 & \ldots & \alpha_{k-1} & \alpha_k & \beta_1 & \ldots & \beta_{k-1} & \beta_k \\ 0 & 1 & \ldots & 0 & 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 & 0 & \ldots & 0 & 0 \\ 1 & 0 & \ldots & 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \ldots & 1 & 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & 0 & 1 & \ldots & 1 & 0 \end{array}\right],$$

with $\mathbf{c}=[1]$. A famous example of linear multistep method is the Numerov method (see, for instance, [57], [60])

$$\begin{aligned} y_n = 2y_{n-1} - y_{n-2} + \frac{h^2}{12}\Big(& f(t_n, y_n) \\ &+ 10 f(t_{n-1}, y_{n-1}) + f(t_{n-2}, y_{n-2})\Big), \end{aligned} \tag{7}$$

which is an order four method corresponding to the GNM with $r=4$, $s=1$, $Y^{[n]}=[y_n]$,

$$y^{[n-1]} = \begin{bmatrix} y_{n-1} \\ y_{n-2} \\ h^2 f(y_{n-1}) \\ h^2 f(y_{n-2}) \end{bmatrix},$$

and reduced tableau (4)

$$\left[\begin{array}{c|cccc} \frac{1}{12} & 2 & -1 & \frac{5}{6} & \frac{1}{12} \\ \hline \frac{1}{12} & 2 & -1 & \frac{5}{6} & \frac{1}{12} \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{array}\right].$$

2) Runge-Kutta-Nyström methods. Runge-Kutta methods of Nyström type (see [57])

$$\begin{aligned} Y_i &= y_{n-1} + c_i h y'_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j), \\ hy'_n &= hy'_{n-1} + h^2 \sum_{j=1}^{s} b'_j f(Y_j), \\ y_n &= y_{n-1} + hy'_{n-1} + h^2 \sum_{j=1}^{s} b_j f(Y_j), \end{aligned} \tag{8}$$

$i=1,\ldots,s$, provide an extension to second order ODEs (1) of Runge–Kutta methods (see, for instance, [5], [66]) which involves the dependence on the approximation to the first derivative. Such methods are GNMs (3) with $r=1$ and Butcher tableau (2)

$$\left[\begin{array}{c|c|c} A & \mathbf{c} & \mathbf{e} \\ \hline \mathbf{b}'^\top & 1 & 0 \\ \hline \mathbf{b}^\top & 1 & 1 \end{array}\right],$$

where $\mathbf{e}$ is the unit vector in $\mathbb{R}^s$, and to the input vectors $y^{[n-1]}=[y_{n-1}]$, $y'^{[n-1]}=[y'_{n-1}]$.

3) Coleman hybrid methods. We now consider the following class of two-step hybrid methods

$$\begin{aligned} Y_i &= (1+c_i)y_{n-1} - c_i y_{n-2} + h^2 \sum_{j=1}^{s} a_{ij} f\left(Y_j\right), \\ y_n &= 2y_{n-1} - y_{n-2} + h^2 \sum_{j=1}^{s} b_j f\left(Y_j\right), \end{aligned} \tag{9}$$

$i = 1, ..., s$, introduced by Coleman in [24], which are GNMs corresponding to the reduced tableau (4)

$$\left[\begin{array}{c|cc} A & \mathbf{e}+\mathbf{c} & -\mathbf{c} \\ \hline \mathbf{b}^\top & 2 & -1 \\ \mathbf{0} & 1 & 0 \end{array}\right]$$

and input vector $y^{[n-1]} = [y_{n-1} \quad y_{n-2}]^\top$.

4) Two-step Runge-Kutta-Nyström methods. The following class of two-step Runge-Kutta-Nyström methods [28]

$$\begin{aligned} Y_i^{[n-1]} &= y_{n-2} + hc_i y'_{n-2} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n-1]}), \\ Y_i^{[n]} &= y_{n-1} + hc_i y'_{n-1} + h^2 \sum_{j=1}^{s} a_{ij} f(Y_j^{[n]}), \\ hy'_n &= (1-\theta)hy'_{n-1} + \theta h y'_{n-2} \\ &\quad + h^2 v'_j f(Y_j^{[n-1]}) + h^2 w'_j f(Y_j^{[n]}), \\ y_n &= (1-\theta)y_{n-1} + \theta y_{n-2} + h \sum_{j=1}^{s} v'_j y'_{n-2} \\ &\quad + h \sum_{j=1}^{s} w'_j y'_{n-1} + h^2 \sum_{j=1}^{s} v_j f(Y_j^{[n-1]}) \\ &\quad + h^2 \sum_{j=1}^{s} w_j f(Y_j^{[n]}). \end{aligned} \tag{10}$$

$i = 1, \ldots, s$, depend on two consecutive approximations to the solution and its first derivative in the grid points, but also on two consecutive approximations to the stage values (i.e. the ones related to the points $t_{n-2} + c_i h$ and the ones corresponding to the points $t_{n-1} + c_i h$, $i = 1, 2, \ldots, s$). Two-step Runge-Kutta-Nyström methods can be represented as GNMs (3) with $r = s + 2$ and $r' = 2$ through the tableau (2)

$$\left[\begin{array}{c|cc|ccc} A & \mathbf{c} & \mathbf{0} & \mathbf{e} & \mathbf{0} & \mathbf{0} \\ \hline \mathbf{w}'^\top & (1-\theta) & \theta & 0 & 0 & \mathbf{v}'^\top \\ \mathbf{0} & 1 & 0 & 0 & 0 & \mathbf{0} \\ \hline \mathbf{w}^\top & \mathbf{w}'^\top\mathbf{e} & \mathbf{v}'^\top\mathbf{e} & (1-\theta) & \theta & \mathbf{v}^\top \\ \mathbf{0} & 0 & 0 & 1 & 0 & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{array}\right],$$

in correspondence of the input vectors

$$y^{[n-1]} = \begin{bmatrix} y_{n-1} \\ y_{n-2} \\ h^2 f(Y^{[n-1]}) \end{bmatrix}, \quad y'^{[n-1]} = \begin{bmatrix} y'_{n-1} \\ y'_{n-2} \end{bmatrix}.$$

II. Accuracy analysis

GNMs theory developed in [44] allows to provide simple effective tools for the convergence analysis of methods, which relies on easy computations related to the their coefficients. Such simple objects are strictly related to the basic definitions of consistency, zero-stability and convergence introduced in [44] which, define, as well known in the literature (refer, for instance, to the monographs [6], [57], [64]), the minimal acceptable demandings on accuracy and stability.

Definition 2.1: A GNM (3) is *preconsistent* if there exist vectors $\mathbf{q}_0$, $\mathbf{q}_1$ and $\mathbf{q}'_1$ such that

$$\begin{aligned} &\mathbf{U}\mathbf{q}_0 = e, \quad \mathbf{W}\mathbf{q}_0 = 0, \quad \mathbf{V}\mathbf{q}_0 = \mathbf{q}_0, \\ &\mathbf{P}\mathbf{q}'_1 + \mathbf{U}\mathbf{q}_1 = \mathbf{c}, \quad \mathbf{R}\mathbf{q}'_1 + \mathbf{W}\mathbf{q}_1 = \mathbf{q}'_1, \\ &\mathbf{Q}\mathbf{q}'_1 + \mathbf{V}\mathbf{q}_1 = \mathbf{q}_0 + \mathbf{q}_1, \end{aligned} \tag{11}$$

where $\mathbf{c}$ is the vector of nodes associated to (3).

Definition 2.2: A preconsistent GNM (3) is *consistent* if there exist vectors $\mathbf{q}_2$ and $\mathbf{q}'_2$ such that

$$\begin{aligned} &\mathbf{C}e + \mathbf{R}\mathbf{q}'_2 + \mathbf{W}\mathbf{q}_2 = \mathbf{q}'_1 + \mathbf{q}'_2, \\ &\mathbf{B}e + \mathbf{Q}\mathbf{q}'_2 + \mathbf{V}\mathbf{q}_2 = \frac{\mathbf{q}_0}{2} + \mathbf{q}_1 + \mathbf{q}_2. \end{aligned} \tag{12}$$

Definition 2.3: A GNM (3) is zero-stable if there exist two real constants C and D such that

$$\|\mathbf{M}_0^m\| \leq mC + D, \quad \forall m = 1, 2, \ldots, \tag{13}$$

being $\mathbf{M}_0$ the block matrix

$$\mathbf{M}_0 = \begin{bmatrix} \mathbf{R} & \mathbf{W} \\ \mathbf{Q} & \mathbf{V} \end{bmatrix}.$$

A criterion equivalent to condition (13) is given in the following theorem, contained in [44].

Theorem 2.1: The following statements are equivalent:

(i) $\mathbf{M}_0$ satisfies the bound (13);
(ii) the roots of the minimal polynomial of the matrix $\mathbf{M}_0$ lie on or within the unit circle and the multiplicity of the zeros on the unit circle is at most two;
(iii) there exist a matrix B similar to $\mathbf{M}_0$ such that

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

As expected, consistency and zero-stability are necessary and sufficient conditions for the convergence of the method (for a formal notion of convergence specialized to GNMs (3), compare [44]). This is proved in the following result.

Theorem 2.2: A GNM method (3) is convergent if and only if it is consistent and zero-stable.

A. Recovering the convergence of classical methods

Using recalled definitions and results, we can easily recover the convergence of the classical numerical methods considered in the previous section. As one can appreciate from the following analysis, each proof is very simple, highlighting the power of the introduced theory of GNMs.

- The Numerov method (7) is consistent with preconsistency and consistency vectors

$$\mathbf{q}_0 = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{q}_1 = \begin{bmatrix} 0 \\ -1 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{q}_2 = \begin{bmatrix} 0 \\ 1/2 \\ 1 \\ 1 \end{bmatrix}.$$

The minimal polynomial associated to the zero-stability matrix of the Numerov method (7) is

$$p(\lambda) = \lambda^2(\lambda - 1)^2,$$

which satisfies the requirement (ii) in Theorem 2.1, i.e. the Numerov method is zero-stable, hence convergent;
- as regards Runge–Kutta–Nyström methods (8), preconsistency and consistency vectors assume the forms

$$\mathbf{q}_0 = [1], \quad \mathbf{q}_1 = \mathbf{q}_2 = [0], \quad \mathbf{q}_1' = [1], \quad \mathbf{q}_2' = [0],$$

and the minimal polynomial of the zero-stability matrix is

$$p(\lambda) = (\lambda - 1)^2,$$

which satisfies the requirement (ii) in Theorem 2.1, hence the method is convergent;
- Coleman hybrid methods (9) are consistent with preconsistency and consistency vectors

$$\mathbf{q}_0 = [1 \quad 1]^\top, \quad \mathbf{q}_1 = [0 \quad -1]^\top, \quad \mathbf{q}_2 = [0 \quad 1/2]^\top.$$

Moreover, the minimal polynomial associated to their zero-stability is

$$p(\lambda) = (\lambda - 1)^2,$$

then they provide a family of zero-stable methods;
- two-step Runge–Kutta–Nyström methods (10) are consistent with preconsistency and consistency vectors

$$\mathbf{q_0} = [1 \quad 1 \quad 0 \quad \dots \quad 0 \quad 0]^\top \in \mathbb{R}^{s+2},$$
$$\mathbf{q_1} = [0 \quad -1 \quad 0 \quad \dots \quad 0 \quad 0]^\top \in \mathbb{R}^{s+2},$$
$$\mathbf{q_2} = [0 \quad 1/2 \quad 1 \quad \dots \quad 1 \quad 1]^\top \in \mathbb{R}^{s+2},$$
$$\mathbf{q_1}' = [1 \quad 1]^\top, \quad \mathbf{q_2}' = [0 \ -1]^\top.$$

The minimal polynomial of their zero-stability matrix is

$$p(\lambda) = \lambda^2(\lambda^2 - (1-\theta)\lambda - \theta)$$

and, therefore, such methods are zero-stable if and only if $-1 < \theta \leq 1$: this restriction on θ recovers the classical result on the zero-stability of two-step Runge–Kutta–Nyström methods (compare [29], [68]).

III. Linear stability analysis

Let us now analyze the linear stability properties of GNMs (3), i.e. we analyze the properties of such methods when applied to scalar linear test equation

$$y'' = -\lambda^2 y, \tag{14}$$

introduced by Lambert and Watson in [67]. Applying GNMs methods (3) to the test equation (14), we obtain

$$Y^{[n]} = -\lambda^2 h^2 \mathbf{A} Y^{[n]} + \mathbf{U} y^{[n-1]}, \tag{15}$$

$$y^{[n]} = -\lambda^2 h^2 \mathbf{B} Y^{[n]} + \mathbf{V} y^{[n-1]}. \tag{16}$$

We set $z = \lambda h$ and $\Lambda = (\mathbf{I} + z^2\mathbf{A})^{-1}$, assuming that z is small enough to make the matrix $\mathbf{I} + z^2\mathbf{A}$ invertible. Then (15) is equivalent to

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

and, together with (16), we obtain

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

where

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

The matrix $\mathbf{M}(z^2)$ is known as *stability matrix* and its characteristic polynomial $p(\omega, z^2)$ is the *stability polynomial* of GNMs, having degree r with respect to ω and coefficients given by rational functions with respect to z^2. Correspondingly, we can provide the notions of periodicity interval and P-stability [71] for GNMs.

Definition 3.1: $(0, H_0^2)$ is a *periodicity interval* for a GNM (3) 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 GNM is *P-stable* if its periodicity interval is $(0, +\infty)$.

P-stability is a minimal stability requirement when approximating numerically the solutions of *periodic stiff* problems as greatly clarified, for instance, in [70] and references therein. Periodic stiff problems have a periodic theoretical solution given by the linear combination of components with dominant short frequencies and components with large frequencies and small amplitudes. Accurately computing such solutions imposes severe restriction on the stepsize in order to accurately catch any oscillation. However, this limit can be efficiently removed when P-stable methods are employed since, for such methods, the choice of the stepsize is completely independent from the values of the frequencies, but it only depends on the desired accuracy [26], [68], [70]. This notion completely parallels that of A-stability for first order ODEs, which is highly relevant for stiff problems, eliminating stepsize restrictions due to stability reasons (see citebutch08,hawa and references therein).

A. Runge-Kutta-Nyström stability

P-stability is an important requirement in the numerical approximation of periodic stiff problems. However, it is not so easy to gain a nice balance between P-stability and high order of convergence. For instance, P-stable linear multistep methods (6) can achieve maximum order 2, as proved in [67]. Moreover, no P-stable one-step symmetric collocation methods exist [25].

As regards Runge-Kutta-Nyström methods (8), many A-stable methods exist, but P-stability is hard to be achieved. Indeed, collocation methods among the family (8), i.e. whose coefficients are given by [57]

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

have only bounded stability intervals and are not P-stable [68].

A better balance between order of convergence and P-stability can be acquired by inheriting good stability properties from Runge-Kutta methods for first order ODES, leading to the so-called family of *indirect* collocation methods [27], [71]. Such methods are generated by applying a collocation Runge-Kutta method (the idea of numerical collocation is well described in [6], [12]–[14], [30], [32]–[34], [37], [45], [48], [49], [51], [57] and references therein) to the first order representation of (1). The properties of indirect collocation methods are totally inherited by those of the corresponding reference collocation method [71]. Hence, the maximum attainable order of convergence is $2s$, where s is the number of internal stages, and it is achieved by Gaussian collocation points; Gaussian methods are also A-stable, while Radau IIA methods have order $2s-1$ and are L-stable. P-stability is achieved in correspondence of Gauss-Legendre collocation points [71]: such methods of order $2s$ and stage order s have been for many years, at the best of our knowledge, the family of P-stable methods with the highest order of convergence. However, the theory of GNMs has allowed to derive higher order P-stable methods, as discussed in [52].

A crucial role in developing high order P-stable methods for (1) has been played by imitating the P-stability properties of Runge-Kutta-Nyström methods on Gauss Legendre points, by enforcing the stability polynomial of a GNM to contain, as a factor, the stability polynomial of a known P-stable method. Such an idea has also been exploited in the setting of first order ODEs, taking into account that Runge-Kutta methods are excellent starting point to derive accurate and highly stable methods: this is the basis of the idea of Runge-Kutta stability (see [1], [2], [6], [9], [64], [72] and references therein), which can be defined as follows. A multivalue method for first order ODEs is *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. In order terms, the corresponding multivalue method shares the same stability properties of the reference Runge-Kutta method.

Following this idea (also compare [8], [18], [31], [64]), we have introduced in [52] an analogous notion of stability for GNMs methods (3), in order to inherit the same stability properties of a reference Runge-Kutta-Nyström method.

Definition 3.3: A GNM method (3) is said to be *Runge-Kutta-Nyström stable* (RKN 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.

Therefore, the corresponding stability properties only depend on the polynomial

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

which is assumed to be the stability polynomial of a P-stable method. Therefore RKN stable GNMs on Gauss-Legendre points are P-stable. Next section shows examples of GNMs sharing the P-stability of Gauss-Legendre methods.

IV. Nordsieck GNMs

In the direction of deriving proper examples of highly stable GNMs (3), we first need to specialize the family of methods, in order to establish which are the quantities that are involved in the multivalue dynamics. In other terms, we a-priori fix the nature of the vector $y^{[n]}$ in (3). An effective choice is generally given by approximating the so-called Nordsieck vector (see [64] and references therein)

$$\begin{bmatrix} y(t_n) \\ hy'(t_n) \\ \vdots \\ h^p y^p(t_n) \end{bmatrix}, \tag{17}$$

where the component $y_i^{[n]}$ 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 always assume $r = p+1$.

As a consequence, the preconsistency and consistency vectors are given by

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

i.e. they are the first three vectors e_1, e_2, e_3 of the canonical basis of R^r. This is a nice property that strongly further simplifies the analysis of convergence of Nordsieck GNMs, as described in the following result [52].

Theorem 4.1: A GLN (3) whose input vector $y^{[n]}$ approximates the Nordsieck vector (17) 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 $\bar{V}$ have modulus strictly less than 1, being $\bar{V}$ the matrix $\widetilde{V}$ deprived of its first two rows.

Theorem 4.1 suggests that the first two columns of the matrices $\mathbf{U}$ and $\mathbf{V}$ play a role in the convergence of a Nordsieck GNM. The remaining ones dictate the order of convergence of the method, as stated in the following theorem.

Theorem 4.2: A GLN method (3) in Nordsieck form has order and stage-order both equal to p if and only if

$$v^{(k+1)} = \sum_{\ell=0}^{k} \frac{e_{k-\ell+1}}{\ell!} - \frac{\mathbf{B}\mathbf{c}^{k-2}}{(k-2)!}, \qquad u^{(k+1)} = \frac{\mathbf{c}^k}{k!} - \frac{\mathbf{A}\mathbf{c}^{k-2}}{(k-2)!}, \tag{18}$$

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

We observe that order conditions (18) also holds true when the order p and stage-order q differs by one, i.e. when $q = p - 1$ (compare [44], [64]).

A. High order P-stable methods

In developing an example of P-stable GNM (3) of Nordsieck type whose order of convergence is higher than that of an existing method having the same computational cost, we suppose that the dimension of the internal stage vector is $s = 1$ and assume as reference the following Runge-Kutta-Nyström of indirect collocation on one single Gauss-Legendre point

$$\begin{aligned} Y &= y_{n-1} + \frac{h}{2}y'_{n-1} + \frac{h^2}{4}f(Y), \\ hy'_n &= hy'_{n-1} + \frac{h^2}{2}f(Y), \\ y_n &= y_{n-1} + hy'_{n-1} + h^2 f(Y), \end{aligned} \tag{19}$$

whose stability polynomial is

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

hence it is P-stable. As regards its accuracy, the order of convergence is equal to 2 and the stage order is 1.

As a consequence, we need to look for a one-stage P-stable GNM of order at least 3, to get a better balance between stability and accuracy. To this purpose,

- we study convergence through Theorem 4.1;
- we impose order 3 through Theorem 4.1;
- we force the stability polynomial to assume the form
$$p(\omega, z^2) = \omega^{r-2}\left(\omega^2 + \frac{2\left(-4+z^2\right)}{4+z^2}\omega + 1\right),$$
to automatically ensure P-stability.

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 $\mathbf{A} = \left[\frac{1}{4}\right]$,

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

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

$$\mathbf{V} = \left[\begin{array}{ccccc} 1 & 1 & & & \\ 0 & 1 & & & \\ 0 & 0 & v_3 & v_4 & v_5 \\ 0 & 0 & & & \\ 0 & 0 & & & \end{array}\right],$$

with

$$v_3 = \left[\begin{array}{c} \frac{-30+64c-37c^2+10c^3-c^4}{24} \\ \frac{-43+76c-30c^2+4c^3}{24} \\ \frac{-4+5c-c^2}{2} \\ c-\frac{5}{2} \\ -1 \end{array}\right],$$

$$v_4 = \left[\begin{array}{c} \frac{4-42c+64c^2-37c^3+10c^4-c^5}{24} \\ \frac{12-67c+76c^2-30c^3+4c^4}{24} \\ \frac{2-6c+5c^2-c^3}{2} \\ 1-\frac{5c}{2}+c^2 \\ -c \end{array}\right],$$

$$v_5 = \left[\begin{array}{c} \frac{2-42c^2+64c^3-37c^4+10c^5-c^6}{48} \\ \frac{16-67c^2+76c^3-30c^4+4c^5}{48} \\ \frac{2-6c^2+5c^3-c^4}{4} \\ \frac{4-5c^2+2c^3}{4} \\ 1-\frac{c^2}{2} \end{array}\right]$$

and $c \approx 0.3754243604533405$ 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 $(0, 1)$.

k	$\|err(20\pi)\|_\infty$	p	fe
3	$5.86 \cdot 10^{-1}$		480
4	$3.99 \cdot 10^{-2}$	3.87	959
5	$2.53 \cdot 10^{-3}$	3.98	1916
6	$1.59 \cdot 10^{-4}$	3.99	3838
7	$9.94 \cdot 10^{-6}$	4.00	7670
8	$6.21 \cdot 10^{-7}$	4.00	15340

TABLE I
NUMERICAL RESULTS FOR 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

k	$\|err(20\pi)\|_\infty$	p	fe
3	$4.47 \cdot 10^{-1}$		477
4	$1.24 \cdot 10^{-1}$	1.98	957
5	$2.82 \cdot 10^{-2}$	1.99	1917
6	$7.05 \cdot 10^{-3}$	1.99	3837
7	$1.76 \cdot 10^{-3}$	2.00	7677
8	$4.41 \cdot 10^{-4}$	2.00	15357

TABLE II
NUMERICAL RESULTS FOR RKN2 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

V. NUMERICAL EVIDENCE

Above order 4 method (denoted as GNM4) is compared with the reference Runge-Kutta-Nyström method (19), denoted as RKN2. Since they are both one-stage methods, they require the same computational cost. Such methods are applied on the periodic stiff Kramarz problem [65]

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

with initial conditions

$$y(0) = [2, -1]^\top, \quad y'(0) = [0, 0]^\top.$$

The eigenvalues of the Jacobian matrix

$$\begin{bmatrix} \mu-2 & 2\mu-2 \\ 1-\mu & 1-2\mu \end{bmatrix}$$

are -1 and $-\mu$. Then, the solution of the problem depends on the two frequencies 1 and $\sqrt{\mu}$. The high frequency component, corresponding to $\sqrt{\mu}$ when $\mu \gg 1$, is eliminated by the initial conditions: the exact solution is indeed $y(t) = [2\cos(t), -\cos(t)]^\top$. 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 results with fixed stepsize

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

for various integer values of k. The results, reported in Tables I and II, confirm the theoretical order of convergence and reveal the superiority of the GNM4 method.

VI. CONCLUSIONS

The paper has reported a selection of novel results on the numerical approximation of initial value problems based on second order ODEs (1) by means of multivalue numerical methods (3) which enables to analyze convergence in an elegant and effective way and compute new methods achieving a better balance between order and stability, as shown. Clearly, this theory opens new paths in different direction, both for other operators (such as partial differential equations [16], [19]–[21], [35], [50], [55], conservative problems [7], [41], [42], [46], [47], integral and fractional equations [4], [10], [11], [15], [17], [23], [30]) and for the development of methods depending on non-constant coefficients and, therefore, useful for oscillatory problems (as in [36], [38], [53], [56], [62], [63], [69]).

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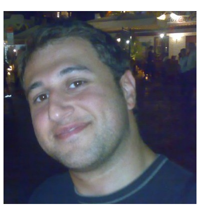

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