Multivalue collocation methods free from order reduction

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Abstract

This paper introduces multivalue collocation methods for the numerical solution of stiff problems. The presented approach does not exhibit the phenomenon of order reduction, typical of collocation based Runge-Kutta methods applied to stiff systems, since the introduced methods have uniform effective order of convergence on the overall integration interval. Examples of methods as well as numerical experiments on a selection of stiff problems are given.

Key words: Stiff problems, multivalue numerical methods, collocation methods, order reduction.

1. Motivational aspects

In this paper, we aim to consider the numerical solution of stiff problems of the general class $y' = f(y)$, which commonly arise from time-dependent partial differential equations discretized along the space variable. The key point in solving stiff problems is that of employing suitable highly stable numerical methods possibly avoiding order reduction phenomena, typical of classical numerical formulae such as Runge-Kutta methods [2]. Even if there is an extensive bibliography regarding the numerical solution stiff problems (we refer, for instance, to the monographs [2, 19, 24, 26] and references therein), this issue still deserves attention, since stiffness is intrinsic in many situations of interest. A gifted contribution on the topic is the paper [36], where the authors provide a modern vision of stiffness, also very well framed in the existing literature.

Stiff problems arise in many relevant mathematical models, such as those describing multiscale problems. *"Stiff equations are multiscale problems"*: this sentence, contained in the first pages of [3], provides an example of stiff equations occurring in the description of coupled physical systems having components which vary on very different time-scales (also see [19, 37] and references therein). This situation is very common, for instance, in the spatial discretization of time-dependent partial differential equations by the method of lines through finite elements or finite differences. In recent times, in many contexts such as Immunology, multiscale models are extensively developed, for instance to support the major challenge of identifying drug targets that efficiently interfere with viral replication in case of influenza [23]. Multiscale modeling provides an ideal framework to combine several aspects such as immune response, pharmacokinetics and comprehensive information on virus-host interactions as diverse cellular processes which can be simulated individually and incorporated as separate modules into a unifying framework.

In summary, improving the numerical treatment of stiff ordinary differential equations can provide a benefit in a wider range of problems and situations of certain interest. As aforementioned, the main gap regarding the existing literature on the numerical treatment of stiff problems is given by the order reduction phenomenon visible in classical Runge-Kutta methods [2], thus the main improvement here provided regards the introduction of numerical methods free from order reduction when applied to stiff problems. This issue is studied in the context of a wide family of methods, i.e. the so-called *multivalue* numerical methods, for which we aim to define a suitable notion of numerical collocation, a methodology which seems particularly suitable to solve stiff problems (see [19] and references therein). In particular, we will introduce and analyze multivalue collocation methods which do not show order reduction phenomenon, as it happens for classical collocation methods, i.e. those based on suitable implicit Runge-Kutta methods. The treatise is organized as follows: Section 2 contains a brief review of methodological aspects regarding the classical idea of numerical collocation and some extensions; Section 3 introduces multivalue numerical methods, for which we look for smooth continuous extensions; Section 4 presents the form of the continuous approximant and its usefulness; Section 5 gives an error analysis leading to the set of uniform order conditions and also focuses on linear stability properties, giving possible order and stability barriers for A-stable multivalue collocation methods; examples of methods are given in Section 6, while numerical experiments are object of Section 7. Some conclusions are given in Section 8.

2. Methodology: a brief review on (modified) collocation methods

As announced, we aim to numerically treat stiff problems by novel collocation-based numerical methods. Collocation [2, 19, 26, 41] is an extensively applied technique based on the idea of approximating the exact solution of a given functional equation with a continuous approximant belonging to a chosen finite dimensional space (desirably chosen coherently with the qualitative behaviour of the solution). Such an approximant usually satisfies interpolation conditions in the grid points and exactly satisfies the equation on a given set of points, the so-called collocation points. We now briefly recall some basic aspects regarding collocation methods, together with some recent modifications developed in the literature.

- *One-step collocation.* In classical one-step collocation methods (see [2, 19, 26]) the collocation function is given by an algebraic polynomial $P_n(t)$, $t \in [t_n, t_{n+1}]$, satisfying

$$P_n(t_n) = y_n, \qquad P_n'(t_n + c_i h) = f(P_n(t_n + c_i h)), \quad i = 1, 2, ..., m,$$

i.e. interpolating the numerical solution in t_n and exactly satisfying the given system in $\{t_n + c_i h,\ i = 1, 2, \ldots, m\}$, where $c_1, c_2, \ldots, c_m$ are given collocation points. The solution in t_{n+1} can then be computed from the function evaluation $y_{n+1} = P_n(t_{n+1})$. Guillou and Soule [18] and Wright [41] independently proved that one step collocation methods form a subset of implicit Runge-Kutta methods,

$$\begin{aligned} y_{n+1} &= y_n + h \sum_{i=1}^{m} b_i f(Y_i), \\ Y_i &= y_n + h \sum_{j=1}^{m} a_{ij} f(Y_j),\ i = 1, 2, \ldots, m, \end{aligned}$$

whose coefficients are given by

$$a_{ij} = \int_0^{c_i} L_j(t)dt, \quad b_i = \int_0^1 L_i(t)dt, \tag{2.1}$$

$i, j = 1, 2, \ldots, m$, being $L_i(t)$ the i-th fundamental Lagrange polynomial over the set of collocation points. The maximum attainable order of such methods is at most $2m$, and it is obtained by using Gaussian collocation points [19, 26], while the uniform order of convergence over the entire integration interval is only m. As a consequence, they suffer from order reduction showing effective order equal to m [2]. Concerning their linear stability properties, it is known that collocation methods based on Gaussian and Lobatto IIIA nodes are A-stable, while the ones based on Radau IIA points are L-stable [2, 19, 26].

- *Perturbed and discontinuous collocation.* As remarked, only some implicit Runge-Kutta methods are of collocation type. The literature on the topic has provided some efforts in order to extend the idea of collocation to a larger class of methods; this operation is useful because the properties of collocation methods (such as order, linear and nonlinear stability) can be derived in a simpler and very elegant way, rather than as it happens outside collocation. An extension of the collocation idea, the so-called perturbed collocation, is due to Norsett and Wanner [32, 33], where the authors proved the equivalence result between the family of perturbed collocation methods and Runge-Kutta methods. Another relevant extension of the collocation principle is given by discontinuous collocation [20], which applies to a larger family rather than collocation.

- *Multistep collocation.* The idea of multistep collocation was first introduced by Lie and Norsett in [29] (also see [18, 19, 28]) and extends the collocation technique to the family of multistep Runge-Kutta method. The collocation polynomial $P_n(t)$ satisfies the following interpolation and collocation conditions:

$$P_n(t_{n-i}) = y_{n-i}, \qquad P_n'(t_n + c_j h) = f(P(t_n + c_j h)),$$

for $i = 0, 1, ..., k-1$ and $j = 1, ..., m$. The numerical solution is then given by $y_{n+1} = P_n(t_{n+1})$. Lie and Norsett [29] proved that the maximum attainable order is $2m + k - 1$. They also proved the existence of $\binom{m+k-1}{k-1}$ nodes allowing superconvergence. However, the corresponding methods are not stiffly stable, while in [19] A-stable methods of highest order $2m + k - 2$ are introduced.

- *Two-step collocation*. Two-step collocation methods extend the collocation idea to the class of two-step Runge-Kutta methods (introduced by Jackiewicz and Tracogna in [25]), pursuing the aim of deriving highly stable collocation-based methods which do not suffer from order reduction. The continuous approximant is given by

$$P(t_n+sh) = \varphi_0(s)y_{n-1}+\varphi_1(s)y_n+h\sum_{j=1}^{m}\Big(\chi_j(s)f(P(t_{n-1}+c_jh))+\psi_j(s)f(P(t_n+c_jh))\Big), \tag{2.2}$$

$s \in [0,1]$. The collocation polynomial (2.2) is expressed as linear combination of the unknown basis functions $\{\varphi_0(s), \varphi_1(s), \chi_j(s), \psi_j(s), j = 1, 2, \ldots, m\}$, to be suitably determined. It is required that the polynomial $P(t_n + sh)$ interpolates the solution in the points t_{n-1} and t_n and collocates it in the points $t_{n-1} + c_ih$, $t_n + c_ih$, $i = 1, 2, \ldots, m$. As proved in [9], this is equivalent to determine the basis functions as unique solution of the order conditions system

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

$s \in [0,1]$, $k = 1, 2, \ldots, 2m+1$. Thus, the maximum attainable order of convergence is $2m+1$, uniformly on the overall integration interval. However, according to the Daniel-Moore theorem [2] (i.e. the maximum attainable order of a m-stage A-stable method is $2m$), such methods cannot be A-stable. Hence, a modification of this idea has been proposed to achieve at least A-stability, leading to the so-called family of almost collocation methods.

- *Almost collocation.* In order to fulfill Daniel-Moore requirement (see [2] and references therein), methods of order $p = m + r$, with $r = 1, 2, \ldots, m$, have to be considered. In two-step collocation methods, this can be made possible by relaxing some order conditions (thus, by removing some interpolation and/or collocation conditions). The corresponding formulae are known in literature as *two-step almost collocation methods*. In [8, 9, 10, 11] many A-stable and L-stable methods have been introduced: such methods do not suffer from the order reduction phenomenon in the integration of stiff systems. This is in contrast to implicit Runge-Kutta methods, whose stage order is only m, suffering from order reduction [2, 19]. However, only low uniform order almost collocation methods have been provided so far in the aforementioned papers.

3. Multivalue numerical methods

Our attention is focused on the family of multivalue numerical methods (see [1, 2, 5, 24] and references therein), i.e. methods transferring a whole vector of information

$$\begin{tikzcd}
y^{[0]} \arrow[r, "\mathcal{G}_h"] & y^{[1]} \arrow[r, "\mathcal{G}_h"] \arrow[d, "\mathcal{F}_h"'] & y^{[2]} \arrow[r, "\mathcal{G}_h"] \arrow[d, "\mathcal{F}_h"'] & \cdots \\
y_0 \arrow[u, "\mathcal{S}_h"] \arrow[r, "\varphi_h"'] & y_1 \arrow[r, "\varphi_h"'] & y_2 &
\end{tikzcd}$$

Figure 1: Dynamics of a multivalue numerical method

from a step to the following one. This vector does not only contain the approximation of the solution of the problem in the step points (as it happens for linear multistep methods and Runge-Kutta methods), but many solution related quantities and evaluations of the vector field along the discretization. The reason why such quantities are considered is essentially twofold: they can be useful and needed for practical purposes (for instance, when not only the positions but also the velocities and other quantities need to be computed, such as in Hamiltonian dynamics [20]); they allow the introduction of additional degrees of freedom in the method which can be exploited to improve classical order and stability barriers.

A multivalue numerical method for the solution of the initial value problem

$$y' = f(y),\ t \geq 0 \qquad y(t_0) = y_0, \tag{3.1}$$

provides a discrete dynamics which is described in Fig. 1.

Indeed, it is characterized by three fundamental maps: a *starting* procedure $\mathcal{S}_h$, for the computation of the missing starting vector $y^{[0]}$; a *forward* procedure $\mathcal{G}_h$, which updates the vector of the approximations at each step point; a *finishing* procedure $\mathcal{F}_h$, that projects each vector of approximations into the corresponding numerical solution, i.e. $y_n = \mathcal{F}_h(y^{[n]})$.

Under some basic hypothesis described in details in [20] (compare Theorem 8.1 in Section XV), one can prove that for any given forward and finishing procedures, there exist a unique starting procedure and a unique one-step method $y_{n+1} = \varphi_h(y_n)$, such that any subdiagram in Fig. 1 referring to a single step commutes. In particular, one can easy recognize a one-step map φ_h that underlies the discrete dynamics of a multivalue methods: it is called *underlying one-step method* and its properties are very important, because they reveal more of the nature of the forward procedure. For instance, in [7], it was proved that for a given G-symplectic method, the underlying one-step method is conjugate symplectic; as well as (see [20]) the underlying one-step method of a symmetric method is symmetric as well.

A widely used representation of multi-value methods is usually given by the family of General Linear Methods (GLMs, compare [2, 24] and references therein)

$$\begin{cases} Y_i^{[n]} = h \sum_{j=1}^{m} a_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} u_{ij} y_j^{[n]}, & i = 1, 2, \ldots, m, \\ y_i^{[n+1]} = h \sum_{j=1}^{m} b_{ij} f(Y_j^{[n]}) + \sum_{j=1}^{r} v_{ij} y_j^{[n]}, & i = 1, 2, \ldots, r, \end{cases} \tag{3.2}$$

provided in correspondence of the uniform grid $\{t_0 + ih, i = 0, 1, \ldots, N\}$, with $h = (T - t_0)/N$. The values $Y_i^{[n]}$ are approximations of $y(t_n + c_i h)$, being $c_1, c_2, \ldots, c_s$ a set of s real numbers (usually belonging to the interval $[0, 1]$); in other terms, $Y_i^{[n]}$ shares the same interpretation of internal stage values as in the case of Runge-Kutta methods.

Representation (3.2) involves the coefficient matrices $\mathbf{A} \in \mathbb{R}^{m \times m}$, $\mathbf{U} \in \mathbb{R}^{m \times r}$, $\mathbf{B} \in \mathbb{R}^{r \times m}$, $\mathbf{V} \in \mathbb{R}^{r \times r}$, which can be collected in the following partitioned $(m + r) \times (m + r)$ Butcher tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right], \tag{3.3}$$

In the remainder of the treatise we will always assume that the vector of the updates $y^{[n]}$ has the so-called Nordsieck form [24]

$$y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix} \approx \begin{bmatrix} y(x_n) \\ hy'(x_n) \\ \vdots \\ h^{r-1} y^{(r-1)}(x_n) \end{bmatrix}, \tag{3.4}$$

i.e. it provides an approximation of the first $r - 1$ scaled derivatives of the solution.

4. Collocation-based Nordsieck methods

We now propose to extend smoothly a multivalue numerical method in GLM form (3.2) and depending on the Nordsieck vector (3.4) by means of a piecewise collocation polynomial of the form

$$P_n(t_n + \vartheta h) = \sum_{i=1}^{r} \alpha_i(\vartheta) y_i^{[n]} + h \sum_{i=1}^{m} \beta_i(\vartheta) f(P_n(t_n + c_i h)), \tag{4.1}$$

with $\vartheta \in [0, 1]$. This representation is provided with respect to the functional basis

$$\{\alpha_i(\vartheta),\ \beta_j(\vartheta),\ i = 1, 2, \ldots, r,\ j = 1, 2, \ldots, m\}$$

to be determined by imposing suitable conditions. In particular, since we aim to provide a collocation polynomial, we impose interpolation conditions of the type

$$P_n(t_n) = y_1^{[n]}, \quad P_n'(t_n) = y_2^{[n]}, \quad \cdots, \quad P_n^{(r-1)}(t_n) = y_{r-1}^{[n]} \tag{4.2}$$

and collocation conditions

$$P_n'(t_n + c_i h) = f(P_n(t_n + c_i h)), \quad i = 1, 2, \ldots, m. \tag{4.3}$$

In other terms, due to the fact that derivatives up to order $r-1$ are interpolated, the global piecewise polynomial generated by multivalue collocation is globally of class C^{r-1}. It is worth observing that most interpolants based on Runge-Kutta methods only have global C^1 continuity, while two-step (almost) collocations methods are globally of class C^0 [15, 16, 17, 22]. The practical value of highly continuous interpolants is visible in many different situations already shown in the existing literature such as scientific visualization [30], functional differential equations with state-dependent delay [21], numerical solution of differential-algebraic equations and nonlinear equations [27, 39, 40], optimal control problems [35], discontinuous initial value problems [16, 38] or, more in general, whenever a smooth dense output is needed [22, 34].

Above interpolation conditions (4.2) on P_n are naturally reflected on the basis functions and, indeed, they are equivalent to

$$\alpha_j(0) = \delta_{j1},\ \alpha_j^{(\nu)}(0) = \delta_{j,\nu+1}, \quad j = 1, 2, \ldots, r, \quad \nu = 1, 2, \ldots, r-1, \tag{4.4}$$

$$\beta_j(0) = \beta_j^{(\nu)}(0) = 0, \quad j = 1, 2, \ldots, m, \quad \nu = 1, 2, \ldots, r-1, \tag{4.5}$$

as well as collocation conditions (4.3) are equivalent to

$$\alpha_j'(c_i) = 0, \quad i = 1, 2, \ldots, r, \quad j = 1, 2, \ldots, m, \tag{4.6}$$

$$\beta_j'(c_i) = \delta_{ij}, \quad i, j = 1, 2, \ldots, m, \tag{4.7}$$

being δ_{ij} the usual Kronecker delta. Above conditions state that each basis function is subject to $m+r$ constraints, hence it is an algebraic polynomial of degree at most $m+r$.

In summary, the collocation polynomial (4.1) is a global smooth extension of class C^{r-1}, of the Nordsieck GLM (3.2) with tableau (3.3) depending on the following matrices

$$\mathbf{A} = \left[\beta_j(c_i)\right]_{i,j=1,\ldots,m}, \quad \mathbf{U} = \left[\alpha_j(c_i)\right]_{i=1,\ldots,m,\ j=1,\ldots,r},$$
$$\mathbf{B} = \left[\beta_j^{(i-1)}(1)\right]_{i=1,\ldots r,\ j=1,\ldots,m}, \quad \mathbf{V} = \left[\alpha_j^{(i-1)}(1)\right]_{i,j=1,\ldots,r}.$$

5. Error and stability analysis

We now aim to analyze the error associated to a multivalue collocation approximant of type (4.1), in order to provide the conditions guaranteeing a uniform approximation of order p to the solution of the differential system. In other terms, a multivalue collocation polynomial (4.1) is required to satisfy

$$P_n(t_n + \vartheta h) = y(t_n + \vartheta h) + O(h^{p+1}), \qquad \vartheta \in [0, 1],$$

i.e., to provide approximations of uniform order on the overall integration interval, which is the main difference with respect to classical collocation based Runge-Kutta methods [2]. Then, the local discretization error associated to a single step of a multivalue collocation method can be defined as the residuum operator

$$\xi_n(t_n + \vartheta h) = y(t_n + \vartheta h) - \sum_{i=1}^{r} \alpha_i(\vartheta) h^{i-1} y^{(i-1)}(t_n) - h \sum_{i=1}^{m} \beta_i(\vartheta) y'(t_n + c_i h), \tag{5.1}$$

with $\vartheta \in [0, 1]$, and y exact solution of the problem. Then, the following result holds.

Theorem 5.1. *A multivalue collocation method given by the approximant $P_n(t_n + \vartheta h)$ in* (4.1)*, $\vartheta \in [0, 1]$, is an approximation of uniform order p to the solution of the well-posed problem* (3.1) *if and only if*

$$\begin{aligned}
&\alpha_1(\vartheta) = 1 \\
&\frac{\vartheta^\nu}{\nu!} - \alpha_{\nu+1}(\vartheta) - \sum_{i=1}^{m} \frac{c_i^{\nu-1}}{(\nu-1)!}\beta_i(\vartheta) = 0, \quad \nu = 1, 2, \ldots, r-1, \\
&\frac{\vartheta^\mu}{\mu!} - \sum_{i=1}^{m} \frac{c_i^{\mu-1}}{(\mu-1)!}\beta_i(\vartheta) = 0, \quad \mu = r, \ldots, p.
\end{aligned} \tag{5.2}$$

Proof: We expand $y(t_n + \vartheta h)$ and $y'(t_n + c_h)$ in Taylor series around t_n and replace them in (5.1), obtaining

$$\begin{aligned}
\xi(t_n + \vartheta_h) = y(t_n) + \vartheta h y'(y_n) + \ldots + \frac{(\vartheta h)^p}{p!} y^{(p)}(t_n) \\
- \alpha_1(\vartheta) y(t_n) - \sum_{j=2}^{r} \alpha_i(\vartheta) h^{i-1} y^{(i-1)}(t_n) \\
- h \sum_{i=1}^{m} \beta_i(\vartheta) \left(y'(t_n) + c_i h y''(t_n) + \ldots + \frac{(c_i h)^{p-1}}{(p-1)!} y^{(p)}(t_n) \right) + O(h^{p+1}).
\end{aligned}$$

Conditions (5.2) arise from annihilating all terms up to order p. □

We can then interpret conditions (5.2) as uniform order conditions for a multivalue collocation methods defined by (4.1). Moreover, from the last theorem, we can also understand which is the uniform order of convergence for a multivalue collocation method.

Corollary 5.1. *The uniform order of convergence for a multivalue collocation method* (4.1) *is $m + r - 1$.*

Proof: The linear system (5.2) is a system of $p + 1$ linearly independent equations in $m + r$ unknowns admitting a unique solution if and only if the number of equations equals that of the unknowns, i.e. when $p = m + r - 1$. □

As well as uniform order conditions, also linear stability plays an important role in this theory. In particular, since we are dealing with collocation - thus implicit - methods, we should require at least A-stability from our novel multivalue collocation integrators. The following result clarifies the restriction on r and s necessary for A-stability.

Theorem 5.2. *An A-stable multivalue collocation method* (4.1) *fulfills the constraint $r \leq m + 1$.*

Proof: A-stable methods are subject to Daniel-Moore theorem (see [2] and references therein), according to which the order of a m-stage method cannot exceed $2m$. Theorem 5.1 says that the uniform order of a multivalue collocation method is $m + r - 1$: this result, merged with Daniel-Moore condition, gives the thesis. □

We can put together all the results proved in this section, in order to state which is maximum attainable order of a A-stable multivalue collocation method.

Corollary 5.2. *The maximum attainable uniform order of convergence for an A-stable multivalue collocation method is* $2m$*.*

Proof: The results is a straightforward consequence of Corollary 5.1 and Theorem 5.2. □

It is worth observing that multivalue collocation methods of maximum uniform order $2m$ totally fills the gap of classical collocation based Runge-Kutta methods on Gauss-Legendre points [26], having order $2m$ only in the grid points. This gap is filled without heightening the computational cost, since the number of internal stages is the same in both cases.

6. Construction of methods

We now aim to provide two examples of multivalue collocation methods, with $m = 1$ and $m = 2$, of maximum uniform order. According to Corollary 5.2, A-stable methods with $m = 1$ have maximum uniform order 2, while those with $m = 2$ have maximum uniform order 4.

In searching for A-stable formulae, we will always need to analyze the properties of the stability matrix [2, 24]

$$\mathbf{M}(z) = \mathbf{V} + z\mathbf{B}(I - z\mathbf{A})^{-1}\mathbf{U}, \tag{6.1}$$

being I the identity matrix in $\mathbb{R}^{m\times m}$.

6.1. One-stage multivalue collocation method

According to Theorem 5.2, A-stability necessarily requires $r \leq m + 1 = 2$ and the maximum order $p = 2$ is achieved with $r = 2$. Thus, we search for A-stable multivalue methods based on (4.1) with $r = 2$ and $m = 1$, i.e.

$$P_n(t_n + \vartheta h) = y_1^{[n]} + \alpha_2(\vartheta)y_2^{[n]} + h\beta_1(\vartheta)f(P_n(t_n + ch)).$$

Order 2 is achieved by solving conditions (5.2) for $p = 2$, i.e.

$$\begin{aligned} &\vartheta - \alpha_2(\vartheta) - \beta_1(\vartheta) = 0 \\ &\frac{\vartheta^2}{2} - c\beta_1(\vartheta) = 0. \end{aligned}$$

This systems leads to

$$\alpha_2(\vartheta) = \vartheta\left(1 - \frac{\vartheta}{2c}\right), \qquad \beta_1(\vartheta) = \frac{\vartheta^2}{2c},$$

which are the basis functions of a general multivalue collocation method (4.1) of order 2, with $r = 2$ and $m = 1$. We now aim to find the values of c such that the corresponding method is A-stable. Thus, we analyze the stability matrix (6.1) corresponding to the Butcher tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} \beta_1(c) & 1 & \alpha_2(c) \\ \hline \beta_1(1) & 1 & \alpha_2(1) \\ \beta_1'(1) & 0 & \alpha_2'(1) \end{array}\right] = \left[\begin{array}{c|cc} \frac{c}{2} & 1 & \frac{c}{2} \\ \hline \frac{1}{2c} & 1 & 1-\frac{1}{2c} \\ \frac{1}{c} & 0 & 1-\frac{1}{c} \end{array}\right]. \tag{6.2}$$

Then, the corresponding stability matrix (6.1) assumes the form

$$\mathbf{M}(z) = \begin{bmatrix} \dfrac{(c^2-1)z-2c}{c(cz-2)} & \dfrac{c(c-1)z-2c+1}{c(cz-2)} \\ -\dfrac{2z}{c(cz-2)} & \dfrac{c(c-2)z-2c-2}{c(cz-2)} \end{bmatrix}$$

and its characteristic polynomial is

$$p(\omega, z) = \omega^2 + p_1(z)\omega + p_0(z),$$

with

$$p_0(z) = \frac{(c-1)^2 z - 2c + 2}{c(cz-2)}, \quad p_1(z) = \frac{(1+2c-c^2)z + 4c - 2}{c(cz-2)}.$$

By performing Schur analysis of this polynomial (for a detailed description of Schur criterion we refer to [8, 26] and references therein), we discover that A-stability is achieved if and only if

$$c \geq 1.$$

6.2. Two-stage multivalue collocation method

We now aim to construct A-stable two-stage methods (4.1) of maximum uniform order. In this case, A-stability requires $r \leq m+1 = 3$ and the maximum order $p = 4$ is achieved with $r = 3$. Hence, we search for A-stable multivalue methods based on (4.1) with $r = 3$ and $m = 2$, i.e.

$$P_n(t_n+\vartheta h) = y_1^{[n]} + \alpha_2(\vartheta) y_2^{[n]} + \alpha_3(\vartheta) y_3^{[n]} + h\left(\beta_1(\vartheta) f(P(t_n + c_1 h)) + \beta_2(\vartheta) f(P(t_n + c_2 h))\right).$$

Order 4 is achieved by solving conditions (5.2) up to $p = 4$, i.e. leading to

$$\alpha_2(\vartheta) = \frac{(c_1+c_2)(3\vartheta - 4c_2)\vartheta^3 + 4c_1^2\vartheta(3c_2^2 - \vartheta^2)}{12c_1^2c_2^2},$$

$$\alpha_3(\vartheta) = \frac{\vartheta^2(6c_1c_2 - 4c_1\vartheta - 4c_2\vartheta + 3\vartheta^2)}{12c_1c_2},$$

$$\beta_1(\vartheta) = \frac{\vartheta^3(3\vartheta - 4c_2)}{12c_1^2(c_1-c_2)}, \qquad \beta_2(\vartheta) = \frac{\vartheta^3(4c_1 - 3\vartheta)}{12c_2^2(c_1-c_2)}.$$

which are the basis functions of a multivalue collocation method (4.1) of order 4, with $r = 3$ and $m = 2$. We now aim to find the values of c_1 and c_2 such that the corresponding

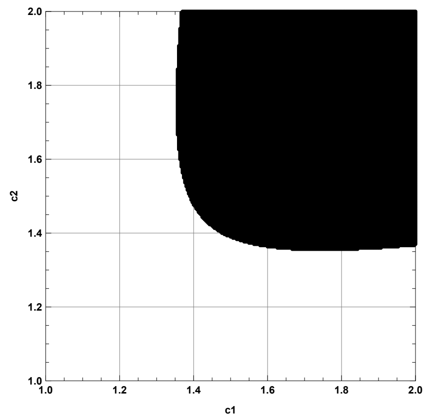

Figure 2: Region of A-stability in the (c_1, c_2) plane for order 4 multivalue methods with $s = 2$ and $r = 3$.

method is A-stable. Thus, we analyze the stability matrix (6.1) corresponding to the Butcher tableau

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{cc|ccc} \beta_1(c_1) & \beta_2(c_1) & 1 & \alpha_2(c_1) & \alpha_3(c_1) \\ \beta_1(c_2) & \beta_2(c_2) & 1 & \alpha_2(c_2) & \alpha_3(c_2) \\ \hline \beta_1(1) & \beta_2(1) & 1 & \alpha_2(1) & \alpha_3(1) \\ \beta_1'(1) & \beta_2'(1) & 0 & \alpha_2'(1) & \alpha_3'(1) \\ \beta_1''(1) & \beta_2''(1) & 0 & \alpha_2''(1) & \alpha_3''(1) \end{array}\right].$$

and perform Schur analysis of its characteristic polynomial. Figure 2 shows the region of A-stability in the (c_1, c_2) plane.

As an example, we choose $c_1 = 3/2$ and $c_2 = 9/5$, obtaining

$$\alpha_2(\vartheta) = \vartheta\left(\frac{55}{486}\vartheta^3 - \frac{91}{243}\vartheta^2 + 1\right), \quad \alpha_3(\vartheta) = \frac{1}{54}\vartheta^2\left(5\vartheta^2 - 22\vartheta + 27\right),$$

$$\beta_1(\vartheta) = -\frac{2}{27}\vartheta^3(5\vartheta - 12), \qquad \beta_2(\vartheta) = \frac{125}{486}\vartheta^3(\vartheta - 2).$$

which is the continuous C^2 extension of uniform order $p = 4$ of the A-stable general linear method

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{cc|ccc} \frac{9}{8} & -\frac{125}{288} & 1 & \frac{233}{288} & \frac{7}{32} \\ \frac{162}{125} & -\frac{3}{10} & 1 & \frac{201}{250} & \frac{27}{125} \\ \hline \frac{14}{27} & -\frac{125}{486} & 1 & \frac{359}{486} & \frac{5}{27} \\ \frac{32}{27} & -\frac{125}{243} & 0 & \frac{80}{243} & \frac{4}{27} \\ \frac{8}{9} & 0 & 0 & -\frac{8}{9} & -\frac{1}{3} \end{array}\right]. \tag{6.3}$$

7. Numerical results

We now provide numerical experiments confirming the theoretical expectations and, in particular, showing that the introduced multivalue collocation methods do not show order reduction when integrating stiff problems as it happens for classical collocation based Runge-Kutta methods [2]. In particular, we aim to show that the effective order of convergence of our methods is $p = 2m$ while, on the contrary, that of Runge-Kutta methods is m. We compare the second order method (6.2), denoted as GLM2 in the remainder of this section, with the second order Gaussian Runge-Kutta method (denoted as RK2)

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

both depending on one single stage and A-stable. We also compare the fourth order method (6.3), next denoted as GLM4, with the fourth order Gaussian Runge-Kutta method (denoted as RK4)

$$\begin{array}{c|cc} \frac{1}{2}-\frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4}-\frac{\sqrt{3}}{6} \\ \frac{1}{2}+\frac{\sqrt{3}}{6} & \frac{1}{4}-\frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

both depending on two stages and A-stable. The comparison occurs in a fixed stepsize environment. We provide both the error in the final point and the observed order of convergence for the following problems:

1. the Prothero-Robinson problem [2]

$$\begin{cases} y'(t) = \lambda(y(t) - \sin(t)) + \cos(t), \quad t \in [0, 10], \\ y(t_0) = y_0, \end{cases}$$

   with $\mathrm{Re}(\lambda) < 0$, employed by several authors [2, 19] to prove order reduction for Runge-Kutta methods;
2. the van der Pol oscillator [19]

$$\begin{cases} y_1' = y_2, & y_1(0) = 2, \\ y_2' = ((1 - y_1^2)y_2 - y_1)/\epsilon, & y_2(0) = -2/3, \end{cases} \tag{7.1}$$

   $t \in [0, 3/4]$, with stiffness parameter ϵ.

As regards the Prothero-Robinson problem, we consider the results originated for different values of the stiffness parameter λ, listed in Tables 1–4. For $\lambda = -10^3$, the problem is not stiff and we see order of convergence $p = 2$ for both RK2 and GLM2 methods, and order $p = 4$ for both RK4 and GLM4 methods. However, when $\lambda = -10^6$, the problem is stiff and the Runge-Kutta method exhibits the order reduction phenomenon, while this is not the case for the multivalue collocation methods GLM2 and GLM4.

As it regards Van der Pol problem, results are presented in Tables 5 and 6, for several values of the parameter ϵ. When the problem is not stiff (i.e. for $\epsilon = 10^{-3}$), both RK4 and GLM4 methods exhibit order of convergence $p = 4$. In the stiff case (i.e. for $\epsilon = 10^{-6}$) RK4 method suffers from order reduction, while the multivalue collocation method GLM4 still preserves order 4.

h	$\lambda = -10^3$		h	$\lambda = -10^6$	
	error	p		error	p
1/10	$6.80 \cdot 10^{-4}$		1/10	$6.81 \cdot 10^{-4}$	
1/20	$1.70 \cdot 10^{-4}$	2.00	1/20	$3.24 \cdot 10^{-4}$	1.07
1/40	$4.25 \cdot 10^{-5}$	2.00	1/40	$1.58 \cdot 10^{-4}$	1.04
1/80	$1.06 \cdot 10^{-5}$	2.00	1/80	$7.83 \cdot 10^{-5}$	1.01

Table 1: Observed errors (in the final step point) and orders of convergence for the RK2 method applied to the Prothero-Robinson problem

h	$\lambda = -10^3$		h	$\lambda = -10^6$	
	error	p		error	p
1/10	$7.16 \cdot 10^{-7}$		1/10	$1.53 \cdot 10^{-9}$	
1/20	$1.75 \cdot 10^{-7}$	2.03	1/20	$3.81 \cdot 10^{-10}$	2.01
1/40	$4.37 \cdot 10^{-8}$	2.00	1/40	$9.19 \cdot 10^{-11}$	2.05
1/80	$1.09 \cdot 10^{-9}$	2.00	1/80	$2.11 \cdot 10^{-11}$	2.12

Table 2: Observed errors (in the final step point) and orders of convergence for the GLM2 applied to the Prothero-Robinson problem

h	$\lambda = -10^3$		h	$\lambda = -10^6$	
	error	p		error	p
1/10	$1.77 \cdot 10^{-4}$		1/10	$1.52 \cdot 10^{-4}$	
1/20	$1.32 \cdot 10^{-5}$	3.75	1/20	$3.84 \cdot 10^{-5}$	1.98
1/40	$7.82 \cdot 10^{-7}$	4.08	1/40	$9.99 \cdot 10^{-6}$	1.94
1/80	$4.78 \cdot 10^{-8}$	4.03	1/80	$2.78 \cdot 10^{-6}$	1.85

Table 3: Observed errors (in the final step point) and orders of convergence for the RK4 method applied to the Prothero-Robinson problem

h	$\lambda = -10^3$ error	$\lambda = -10^3$ p	h	$\lambda = -10^6$ error	$\lambda = -10^6$ p
$1/10$	$2.54 \cdot 10^{-8}$		$1/10$	$2.41 \cdot 10^{-8}$	
$1/20$	$8.29 \cdot 10^{-10}$	4.94	$1/20$	$7.50 \cdot 10^{-10}$	5.01
$1/40$	$2.83 \cdot 10^{-11}$	4.87	$1/40$	$2.21 \cdot 10^{-11}$	5.08
$1/80$	$1.05 \cdot 10^{-12}$	4.75	$1/80$	$7.06 \cdot 10^{-13}$	4.97

Table 4: Observed errors (in the final step point) and orders of convergence for the GLM4 method applied to the Prothero-Robinson problem

h	$\epsilon = 10^{-3}$ error	$\epsilon = 10^{-3}$ p	h	$\epsilon = 10^{-6}$ error	$\epsilon = 10^{-6}$ p
$1/2^6$	$2.25 \cdot 10^{-4}$		$1/2^6$	$1.49 \cdot 10^{-3}$	
$1/2^7$	$1.68 \cdot 10^{-5}$	3.74	$1/2^7$	$3.71 \cdot 10^{-4}$	2.01
$1/2^8$	$1.11 \cdot 10^{-6}$	3.93	$1/2^8$	$8.84 \cdot 10^{-5}$	2.07
$1/2^9$	$7.02 \cdot 10^{-8}$	3.98	$1/2^9$	$1.87 \cdot 10^{-5}$	2.24

Table 5: Observed errors (in the final step point) and orders of convergence for the RK4 method applied to van der Pol problem

h	$\epsilon = 10^{-3}$ error	$\epsilon = 10^{-3}$ p	h	$\epsilon = 10^{-6}$ error	$\epsilon = 10^{-6}$ p
$1/2^6$	$9.93 \cdot 10^{-5}$		$1/2^6$	$1.25 \cdot 10^{-4}$	
$1/2^7$	$5.30 \cdot 10^{-6}$	4.23	$1/2^7$	$5.97 \cdot 10^{-6}$	4.39
$1/2^8$	$2.93 \cdot 10^{-7}$	4.18	$1/2^8$	$2.88 \cdot 10^{-7}$	4.37
$1/2^9$	$1.61 \cdot 10^{-8}$	4.18	$1/2^9$	$1.20 \cdot 10^{-8}$	4.58

Table 6: Observed errors (in the final step point) and orders of convergence for the GLM4 method applied to van der Pol problem

8. Conclusions

We have introduced a theory of multivalue collocation methods in comparison with classical collocation based Runge-Kutta methods. The main issue we achieve by multivalue collocation methods is the lack of order reduction, which is typical of Runge-Kutta methods. Numerical experiments confirm that multivalue collocation methods converge with stage order equal to their order, also in presence of stiffness. For stiff problems, Gaussian Runge-Kutta methods converge with order m, being m the number of internal stages, even if they have theoretical order equal to $2m$. It is also worthwhile mentioning that both multivalue and Runge-Kutta collocation methods require the same computational effort; moreover, stability properties are also the same, since both multivalue and Runge-Kutta collocation methods are A-stable. Future issues of this research will regard the adaptation of this technique to continuous approximants based on non-polynomial basis, especially suitable for the numerical solution of periodic stiff problems [19], also belonging to the numerical discretization of PDEs generating periodic wavefronts [4, 12, 13, 14] and the implementation in a variable stepsize-variable order environment.

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