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Highly stable multivalued collocation methods

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Abstract. The paper is focused on the development of A-stable collocation based multivalued methods for stiff problems. These methods are dense output extensions of discrete multivalued methods, since the solution is approximated by a piecewise collocation polynomial with high global regularity. The underlying multivalued method is assumed to be diagonally implicit and with uniform order of convergence, thus it does not suffer from order reduction, as it happens for classical one-step collocation methods. The effectiveness of the approach is also confirmed by the numerical evidence.

1. Introduction

In this paper, we aim to consider the numerical solution of well-posed initial value problems based on ordinary differential equations (ODEs)

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

with $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$. The employed methodology relies on the employ of the so-called *multivalued numerical methods*, providing a multivalued extension of Runge-Kutta methods. In other terms, these methods update a vector of solution related informations along the grid; this vector does not only contain the approximation of the solution of the problem in the step points, but also other related quantities. This idea allows to simultaneously approximate many needed quantities as well as to involve a larger number of degrees of freedom for better order and stability barriers in comparison with the usual one-step or multistep cases. A comprehensive treatise on the topic can be found in the monographs [3, 66], while the extension to second order problems is object of [37, 39, 40, 52, 55]; the employ of multivalued methods as geometric numerical integrators is discussed in [4, 5, 17, 35, 36, 38, 42, 43].

Recently, in [57], the authors have introduced the idea of multivalued collocation, extending the classical idea of one-step collocation. Collocation is a 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, chosen coherently with the properties of the solution. This approximant satisfies interpolation conditions in the grid points and exactly satisfies the equation on a given set of points, called collocation points.



The classical idea of collocation belongs to one-step methods and is first presented in the papers by Guillon and Soule [62] and Wright [82]. In correspondence of the uniform grid $\mathcal{I}_h = \{t_0 + ih, i = 0, 1, \dots, N\}$, with $h = (T - t_0)/N$, the collocation extension of a one-step method is a polynomial exactly interpolating the numerical solution in t_n and satisfies the system

$$P'_n(t_n + c_i h) = f(P_n(t_n + c_i h)), \quad i = 1, 2, \dots, m,$$

where c_1, c_2, \dots, c_m are the collocation points. The solution in t_{n+1} is computed from the function evaluation $y_{n+1} = P_n(t_{n+1})$. Collocation methods are a class of implicit Runge-Kutta methods. Other extension of the collocation ideas outside implicit methods led to perturbed and discontinuous collocation methods [73, 74] and to multistep collocation methods [69, 70].

One-step collocation methods suffers from order reduction when applied to stiff problems [3, 63]. An attempt to remove this phenomenon has been given in [41, 45, 46, 51], where two-step *almost collocation methods* have been introduced. However A-stable two-step almost collocation methods are not of maximal order. In [57], the authors have obtained A-stable methods of maximal order when applied to stiff problems.

In this paper we aim to provide the collocation extension of A-stable diagonally implicit multivalued methods. After a brief introduction on dense output multivalued methods based on collocation, given in Section 2. The construction of A-stable diagonally implicit multivalued methods based on collocation is presented in Section 3. A numerical evidence is shown in Section 4. Some conclusions are given in Section 5.

2. Dense output multivalued methods

Multivalued methods can be expressed in the general linear methods (GLM) form on the uniform grid \mathcal{I}_h , in the following form

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

$n = 0, \dots, N$, where m is the number of internal stages and r is the number of external stages, $\mathbf{c} = [c_1, c_2, \dots, c_m]^T$ is the abscissa vector and $\mathbf{A} = [a_{ij}]$, $\mathbf{U} = [u_{ij}]$, $\mathbf{B} = [b_{ij}]$ and $\mathbf{V} = [v_{ij}]$ are four coefficient matrices, with:

$$\mathbf{A} \in \mathbb{R}^{m \times m}, \quad \mathbf{U} \in \mathbb{R}^{m \times r}, \quad \mathbf{B} \in \mathbb{R}^{r \times m}, \quad \mathbf{V} \in \mathbb{R}^{r \times r}.$$

Following [57], we assume that the vector of internal stages is in Nordsieck form

$$y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix} \approx \begin{bmatrix} y(x_n) \\ hy'(x_n) \\ \vdots \\ h^{r-1}y^{(r-1)}(x_n) \end{bmatrix}. \quad (3)$$

Correspondingly, the collocation extension has the form of a piecewise collocation polynomial

$$P_n(t_n + \theta h) = \sum_{i=1}^r \alpha_i(\theta) y_i^{[n]} + h \sum_{i=1}^m \beta_i(\theta) f(P_n(t_n + c_i h)), \quad \theta \in [0, 1], \quad (4)$$

providing a dense approximation to the solution of (1). The computation of (4) relies on the following interpolation

$$P_n(t_n) = y_1^{[n]}, \quad P'_n(t_n) = y_2^{[n]}, \quad \dots \quad P_n^{(r-1)}(t_n) = y_{r-1}^{[n]},$$

and collocation conditions

$$P'_n(t_n + c_i h) = f(P_n(t_n + c_i h)), \quad i = 1, 2, \dots, m.$$

The underlying multivalued method depends on the coefficient matrices

$$\begin{aligned} \mathbf{A} &= [\beta_j(c_i)]_{i,j=1,\dots,m}, & \mathbf{U} &= [\alpha_j(c_i)]_{i=1,\dots,m,j=1,\dots,r}, \\ \mathbf{B} &= [\beta_j^{(i-1)}(1)]_{i=1,\dots,m,j=1,\dots,r}, & \mathbf{V} &= [\alpha_j^{(i-1)}(1)]_{i,j=1,\dots,r}. \end{aligned}$$

Remark 1. Let us discuss the global regularity of the piecewise approximant (4). We first observe that it is globally of class C^{r-1} while most interpolants based on Runge-Kutta methods only have global C^1 continuity [59, 60, 61, 65]. The practical value of highly continuous interpolants is visible in many different situations already shown in the existing literature such as scientific visualization [72], functional differential equations with state-dependent delay [64], numerical solution of differential-algebraic equations and nonlinear equations [68, 81], optimal control problems [78], discontinuous initial value problems [60, 79, 80] or, more in general, whenever a smooth dense output is needed [65, 75].

We, now, recall some important results regarding the accuracy of the method [57].

Theorem 2. A multivalued collocation method given by the approximation $P_n(t_n + \theta h)$ in (4), $\theta \in [0, 1]$, is an approximation of uniform order p to the solution of the well-posed problem (1) if and only if

$$\alpha_1(\theta) = 1 \tag{5}$$

$$\frac{\theta^\nu}{\nu!} - \alpha_{\nu+1}(\theta) - \sum_{i=1}^m \frac{c_i^{\nu-1}}{(\nu-1)!} \beta_i(\theta) = 0, \quad \nu = 1, \dots, r-1, \tag{6}$$

$$\frac{\theta^\nu}{\nu!} - \sum_{i=1}^m \frac{c_i^{\nu-1}}{(\nu-1)!} \beta_i(\theta) = 0, \quad \nu = r, \dots, p. \tag{7}$$

Corollary 3. The uniform order of convergence for a multivalued collocation method (4) is $m + r - 1$.

Theorem 4. An A -stable multivalued collocation method (4) fulfills the constraint $r \leq m + 1$.

Theorem 5. The order conditions in (5)-(7) are equivalent to:

$$\alpha_j(0) = \delta_{j1}, \quad \alpha_j^{(\nu)}(0) = \delta_{j,\nu+1}, \quad j = 1, 2, \dots, r, \quad \nu = 1, 2, \dots, r-1, \tag{8}$$

$$\beta_j(0) = \beta_j^{(\nu)}(0) = 0, \quad j = 1, 2, \dots, m, \quad \nu = 1, 2, \dots, r-1, \tag{9}$$

$$\alpha'_j(c_i) = 0, \quad i = 1, 2, \dots, r, \quad j = 1, 2, \dots, m, \tag{10}$$

$$\beta'_j(c_i) = \delta_{ij}, \quad i, j = 1, 2, \dots, m, \tag{11}$$

being δ_{ij} the usual Kronecker delta.

3. Construction of diagonally implicit methods

We want to present an example of multivalued collocation methods with $m = 2$ and lower triangular coefficient matrix \mathbf{A} , so we have to determine the functional basis $\{\beta_j(\theta), j = 1, \dots, m\}$ such that $\beta_j(c_i) = 0$ for $i > j$, so:

$$\beta_j(\theta) = \omega_j(\theta) \prod_{k=1}^{j-1} (\theta - c_k), \quad j = 1, \dots, m, \quad (12)$$

where $\omega_j(\theta)$ is a polynomial of degree $r - m + 1$:

$$\omega_j(\theta) = \sum_{k=0}^{r-m+1} \mu_k^{(j)} \theta^k, \quad (13)$$

To achieve the purpose, we have to relax some of the collocation conditions. We observe that $\beta_j(\theta), j = 1, \dots, m$, are polynomial of degree r and conditions (6) permit to compute the functions $\alpha_i(\theta), i = 1, \dots, r$, from $\beta_j(\theta)$. In the remainder of the treatise, we fix $r = m + 1$. The parameters $\mu_k^{(j)}$ are free parameters which can be chosen by imposing conditions (7) for some values of ν or can be found in order to obtain A-stable methods.

The construction of A-stable methods relies on the analysis of the stability matrix:

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

where I is the identity matrix in $\mathbb{R}^{m \times m}$. In particular, we are interested in the computation of the roots of the stability function of the method

$$p(\omega, z) = \det(\omega I - \mathbf{M}(z)).$$

This roots have to lie in the unit circle for all $z \in \mathbb{C}$ such that $\operatorname{Re}(z) \leq 0$. By the maximum principle, this situation holds true if the denominator of $p(\omega, z)$ does not have poles in the negative half plane \mathbb{C}_- and if the roots of the $p(\omega, iy)$ are in the unit circle for all $y \in \mathbb{R}$. The last condition can be verified using the following Schur criterion.

We present an example of A-stable methods with $m = 2$ and $r = 3$, so $\omega_j(\theta)$ are polynomial of degree 2. The uniform order of those methods is 3. We consider

$$P_n(t_n + \vartheta h) = y_1^{[n]} + \alpha_2(\vartheta)y_2^{[n]} + \alpha_3(\vartheta)y_3^{[n]} + (\beta_1(\vartheta)f(P(t_n + c_1h)) + \beta_2(\vartheta)f(P(t_n + c_2h))).$$

The Butcher tableau of the considered methods is given by

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

Some values for the parameters $\mu_k^{(j)}$ have been chosen by imposing the condition (7) for $\nu = r$

$$\begin{aligned} \mu_0^{(1)} &= \frac{c_2^2}{c_1}, \mu_0^{(2)} = -\frac{c_2^2}{c_1^2} \mu_0^{(1)}, \\ \mu_2^{(1)} &= -\frac{c_2^2}{c_1^2} \mu_1^{(2)} - \frac{-1 + 3c_1^2 \mu_3^{(1)}}{3c_1}, \quad \mu_2^{(2)} = -\frac{-1 + 3c_1^2 \mu_3^{(1)}}{3c_2^2}. \end{aligned}$$

The remaining ones have been chosen by performing the Schur analysis of the characteristic polynomial of the stability matrix corresponding to the aforementioned Butcher tableau, obtaining

$$\mu_0^{(2)} = 0, \quad \mu_1^{(2)} = 0, \quad \mu_3^{(1)} = -\frac{-c_1 + 4c_2}{3c_1(c_1^2 - 4c_1c_2 + 3c_2^2)},$$

so

$$\alpha_2(\vartheta) = \frac{-4\vartheta^3 + 3\vartheta^2(c_1 + c_2) + 3c_1\vartheta(c_1 - 3c_2)}{3c_1(c_1 - 3c_2)}, \quad \alpha_3(\vartheta) = \frac{2\vartheta^3 + 3\vartheta^2(c_2 - c_1)}{6(3c_2 - c_1)}, \quad (14)$$

$$\beta_1(\vartheta) = \frac{\vartheta^2(\vartheta(c_1 - 4c_2) + 3c_2^2)}{3c_1(c_1^2 - 4c_1c_2 + 3c_2^2)}, \quad \beta_2(\vartheta) = \frac{\vartheta^2(\vartheta - c_1)}{c_1^2 - 4c_1c_2 + 3c_2^2}.$$

Figure 1 shows the corresponding region of A-stability in the (c_1, c_2) plane, obtained from the Schur analysis of the collocation method with piecewise approximant (4) and basis functions (14).

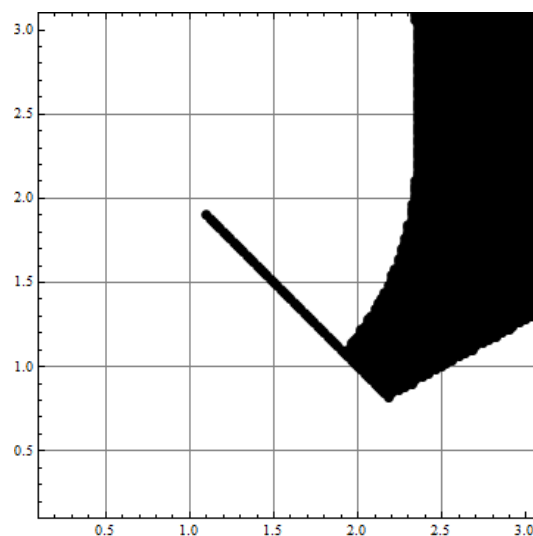


Figure 1. Region of A-stability in the (c_1, c_2) plane.

As an example, we choose $c_1 = 22/10$ and $c_2 = 9/10$, obtaining

$$\alpha_2(\vartheta) = \frac{1}{33}\vartheta(40\vartheta^2 - 93\vartheta + 33), \quad \alpha_3(\vartheta) = \frac{1}{30}\vartheta^2(20\vartheta - 39),$$

$$\beta_1(\vartheta) = \frac{1}{429}\vartheta^2(140\vartheta - 243), \quad \beta_2(\vartheta) = -\frac{4}{13}\vartheta^2(5\vartheta - 11),$$

which is the continuous C^2 extension of uniform order $p = 3$ of the A-stable diagonally implicit

multivalued method with Butcher array

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{cc|ccc} \frac{11}{15} & 0 & 1 & \frac{22}{15} & \frac{121}{150} \\ -\frac{243}{1100} & \frac{81}{50} & 1 & -\frac{549}{1100} & -\frac{567}{1000} \\ \hline -\frac{103}{429} & \frac{24}{13} & 1 & -\frac{20}{33} & -\frac{19}{30} \\ -\frac{2}{13} & \frac{28}{13} & 0 & -1 & -\frac{3}{5} \\ \frac{118}{143} & -\frac{32}{13} & 0 & \frac{18}{11} & \frac{7}{5} \end{array} \right]. \quad (15)$$

4. Numerical evidence

Let us now present the numerical evidence arising from the application of the diagonally implicit collocation-based multivalued method (15) to the Prothero-Robinson problem [3, 63]

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

with $\text{Re}(\lambda) < 0$. The purpose of the experiment is the confirmation of the uniform order 3 of convergence of the method (15), also when the problem is stiff, i.e., when $|\text{Re}(\lambda)| \gg 1$. This is in contrast with classical collocation based Runge-Kutta methods, suffering from order reduction [3]. The method, hereinafter denoted as GLM2, is compared with the two-stage Gaussian Runge-Kutta method (denoted as RK2)

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

which is A-stable, of order 4 and uniform order 2. The comparison is provided in a fixed stepsize environment and shows both the error in the final point and the observed orders of convergence. As shown in Tables 1 and 2, for $\lambda = -10^6$, the problem is stiff and the Runge-Kutta method exhibits order reduction, while this is not the case for GLM2. Actually, GLM2 converges even with one order more, since for the specific problem the leading error term annihilates.

5. Conclusions

In this paper we have introduced diagonally implicit multivalued collocation methods suited to solve stiff problems without exhibiting any order reduction phenomenon. The methods are A-stable and, in comparison with classical collocation based methods, they appear to be more efficient when applied to stiff problems, due to their higher uniform order of convergence. Future issues of this work regard the extension of the idea to other kind of problem such as stochastic differential equations [18, 19, 25, 48], fractional differential equations [2, 11, 14, 20, 34], partial differential equations [12, 24, 47, 49, 53, 56], Volterra integral equations [6, 7, 8, 9, 10, 13, 15, 21, 23, 29, 30, 31, 33], oscillatory problems [26, 27, 28, 32, 50, 54, 58, 71, 77, 76], as well as to the development of algebraically stable high order collocation based multivalued methods [22, 44].

h	$\lambda = -10^6$	
	error	p
1/10	$1.51 \cdot 10^{-7}$	
1/20	$9.21 \cdot 10^{-9}$	4.03
1/40	$5.69 \cdot 10^{-10}$	4.02
1/80	$3.45 \cdot 10^{-11}$	4.04

Table 1. Observed errors (in the final step point) and orders of convergence for the GLM2 applied to the Prothero-Robinson problem

h	$\lambda = -10^6$	
	error	p
1/10	$1.52 \cdot 10^{-4}$	
1/20	$3.84 \cdot 10^{-5}$	1.98
1/40	$9.99 \cdot 10^{-6}$	1.94
1/80	$2.78 \cdot 10^{-6}$	1.85

Table 2. Observed errors (in the final step point) and orders of convergence for the RK4 method applied to the Prothero-Robinson problem

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