

Review

Multivalued Collocation Methods for Ordinary and Fractional Differential Equations

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Abstract: The present paper illustrates some classes of multivalued methods for the numerical solution of ordinary and fractional differential equations. In particular, it focuses on two-step and mixed collocation methods, Nordsieck GLM collocation methods for ordinary differential equations, and on two-step spline collocation methods for fractional differential equations. The construction of the methods together with the convergence and stability analysis are reported and some numerical experiments are carried out to show the efficiency of the proposed methods.

Keywords: ordinary differential equations; fractional differential equations; multistep methods; collocation; convergence; stability

MSC: 65L05; 65L20; 26A33



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1. Introduction

Numerical collocation is an effective technique for the approximation of solutions to a given functional equation by means of a continuous approximate belonging to a finite dimensional space spanned by functions chosen in accordance with the qualitative behavior of the exact solution. This idea has successfully been applied in several contexts (a very brief and far from being extensive, list of contributions in the existing literature can be found in [1–36] and references therein).

In this paper, we aim to collect some of our recent results showing the effectiveness of collocation in two selected cases:

- Firstly, the case of stiff differential problems [1–3,37,38], commonly arising from spatially discretized time-dependent partial differential equations. This problem commonly exposes numerical schemes to the order reduction phenomena, typically characterizing low stage-order methods such as Runge–Kutta methods on Gaussian collocation points [1]. It is worth highlighting that improving the numerics for stiff problems has a direct impact on the numerical treatment of a wide class of problems that is interesting in several applications. A relevant case is given, for instance, by multiscale problems: Quoting from [39], “*Stiff equations are multiscale problems*” and this situation typically characterizes coupled physical systems whose components vary on different time-scales. It is the case, for instance, of epidemiological models for influenza or pandemics (see, for instance, refs. [40–42] and references therein), since multiscale models are an ideal framework to simultaneously simulate several processes such as immune response, pharmacokinetics, and interactions between virus and host.

Our proposal to remove order reduction in providing approximate solutions to stiff problems is to employ multivalued numerical methods based on numerical collocation.

These methods are free from order reduction, as it happens for classical collocation methods. This topic is the subject of Sections 2 and 3;

- Secondly, the case of fractional differential problems, representing a fundamental tool to model anomalous diffusion [43], material hereditariness, viscoelastic materials [44], and heat conduction [45]. For these problems, the analytical solution is generally not available and the numerical treatment is not an easy task, due to the lack of smoothness of the analytical solution and general methods for Ordinary Differential Equations (ODEs), applied to Fractional Differential Equations (FDEs), generally exhibit low order of convergence, e.g., predictor-corrector methods [46]. Therefore ad hoc numerical methods should be formulated to obtain a higher degree of accuracy, as for example fractional linear multistep methods [47], a class of product integration methods [48]. In this scenario, an important role is played by collocation methods, as for example B-spline wavelets collocation [28], Chebychev collocation [49], spectral collocation [16,33,50,51], and non-polynomial collocation [25]. In this paper, we focus on spline collocation methods, which were first introduced by Blank [52], however the main contribution to the development and analysis of these methods has been given in [19,29,30,53]. More recently, multivalued spline collocation methods have been proposed [18,20,54]. This topic is the subject of Section 4.

2. Multivalued Collocation Methods

Multivalued methods for the numerical solution of ODEs [1,37,55–57]:

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

with $y : [t_0, T] \rightarrow \mathbb{R}^d$ $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$, and have the form:

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

where $t_n = t_0 + nh, n = 0, 1, \dots, N$ are the grid points and $h = (T - t_0)/N$ is a fixed stepsize. The matrices:

$$\mathbf{A} = [a_{ij}] \in \mathbb{R}^{m \times m}, \quad \mathbf{U} = [u_{ij}] \in \mathbb{R}^{m \times r}, \quad \mathbf{B} = [b_{ij}] \in \mathbb{R}^{r \times m}, \quad \mathbf{V} = [v_{ij}] \in \mathbb{R}^{r \times r} \tag{3}$$

are the coefficients of the methods and the vector $\mathbf{c} = [c_1, c_2, \dots, c_m]^T$ is called the abscissa vector. The parameters c_1, c_2, \dots, c_m are usually included in $[0, 1]$, but in some cases can be taken outside this interval in order to obtain *A*-stability (see for example Figure 1).

The values $Y_i^{[n]} \in \mathbb{R}^d$ are called internal stages and provide an approximation to $y(t_n + c_i h)$, while $y_i^{[n]} \in \mathbb{R}^d$ are called external stages, and each $y_i^{[n]}$ provides an approximation to a linear combination of the derivatives of y at the point t_n . The number of internal stages m and the number of external stages r , influence the order of convergence and the computational cost of the method, as will be shown later for some classes of methods.

As usual, the coefficient matrices of the multivalued numerical method (2) can be gathered in the Butcher tableau:

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

Collocation multivalued numerical methods represent a continuous extension of multivalued numerical methods in the GLM (General Linear Method) form (2), by means of following piecewise collocation polynomial:

$$P_n(t_n + \theta h) = \sum_{i=1}^r \alpha_i(\theta)y_i^{[n]} + h \sum_{i=1}^m \beta_i(\theta)f(P_n(t_n + c_i h)), \quad \theta \in [0, 1], \tag{5}$$

and by interpreting the internal stages in (2) as $Y_i^{[n]} = P_n(t_n + c_i h)$. In (5), the polynomials $\alpha_i(\theta)$ and $\beta_i(\theta)$ have a degree equal to the order p of the method and are usually computed by solving continuous order conditions, as will be described in the following.

Several kind of multivalued collocation methods have been introduced so far, with a different form for the vector of external stages. We will describe in the next two subsections two different choices which lead to two-step collocation methods and Nordsieck GLM collocation methods.

2.1. Two-Step Collocation Methods

Two-step collocation methods have been introduced in [5] and have the form:

$$\begin{aligned} Y_i^{[n]} &= \varphi_0(c_i)y_{n-1} + \varphi_1(c_i)y_n + h \sum_{j=1}^m (\psi_j(c_i)f(Y_j^{[n]}) + \chi_j(c_i)f(Y_j^{[n-1]})) \quad i = 1, 2, \dots, m, \\ y_{n+1} &= \varphi_0(1)y_{n-1} + \varphi_1(1)y_n + h \sum_{j=1}^m (\psi_j(1)f(Y_j^{[n]}) + \chi_j(1)f(Y_j^{[n-1]})). \end{aligned} \tag{6}$$

with a collocation polynomial defined by:

$$P_n(t_n + \theta h) = \varphi_0(\theta)y_{n-1} + \varphi_1(\theta)y_n + h \sum_{j=1}^m (\psi_j(\theta)f(P(t_n + c_j h)) + \chi_j(\theta)f(P(t_{n-1} + c_j h))), \tag{7}$$

with $\theta \in [0, 1]$ and $Y_j^{[n]} = P(t_n + c_j h)$, $Y_j^{[n-1]} = P(t_{n-1} + c_j h)$.

We observe that such methods can be viewed as multivalued collocation methods (2)–(5), by choosing $r = m + 2$,

$$\begin{aligned} \alpha_1(\theta) &= \varphi_1(\theta), & \alpha_2(\theta) &= \varphi_0(\theta), \\ \alpha_{2+i}(\theta) &= \chi_i(\theta), & \beta_i(\theta) &= \psi_i(\theta) \quad i = 1, \dots, m \end{aligned}$$

and

$$y^{[n]} = \begin{bmatrix} y_n \\ y_{n-1} \\ hF(Y^{[n-1]}) \end{bmatrix} \in \mathbb{R}^{m+2}, \tag{8}$$

where,

$$Y^{[n]} = \begin{bmatrix} Y_1^{[n]} \\ \vdots \\ Y_m^{[n]} \end{bmatrix}, \quad F(Y^{[n]}) = \begin{bmatrix} f(Y_1^{[n]}) \\ \vdots \\ f(Y_m^{[n]}) \end{bmatrix}. \tag{9}$$

With the choice (8) for the external approximation vector, the collocation polynomial (5) is a global smooth extension of the GLM (2) with tableau (4) given by the following matrices:

$$\begin{aligned} \mathbf{A} &= [\beta_j(c_i)]_{i,j=1,\dots,m} \in \mathbb{R}^{m \times m}, & \mathbf{U} &= [\alpha_j(c_i)]_{i=1,\dots,m,j=1,\dots,r} \in \mathbb{R}^{m \times r}, \\ \mathbf{w} &= [\alpha_j(1)]_{j=1,\dots,r} \in \mathbb{R}^r, & \mathbf{v} &= [\beta_j(1)]_{j=1,\dots,m} \in \mathbb{R}^m \\ \mathbf{B} &= \begin{bmatrix} \mathbf{v}^T \\ \mathbf{0} \\ \mathbf{I} \end{bmatrix} \in \mathbb{R}^{r \times m}, & \mathbf{V} &= \begin{bmatrix} \mathbf{w}^T \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \in \mathbb{R}^{r \times r}, \end{aligned}$$

where \mathbf{I} is the identity matrix of dimension m and $\mathbf{0}$ is a zero matrix or vector of suitable dimensions.

Order conditions can be formalized by the following theorem [5].

Theorem 1. *A multivalued collocation method (2) with collocation polynomial in (5) and vector of external stages defined by (8) is an approximation of uniform order p to the solution of the well-posed problem approximates in the solution of (1) with uniform order p , if the following conditions are satisfied:*

$$\frac{\theta^v}{v!} - \frac{(-1)^v}{v!} \alpha_2(\theta) - \sum_{i=1}^m \left(\frac{(c_i - 1)^{v-1}}{(v-1)!} \alpha_{2+i}(\theta) + \frac{(c_i)^{v-1}}{(v-1)!} \beta_i(\theta) \right) = 0, \quad v = 1, \dots, p. \tag{10}$$

The maximum attainable order is $p = m + r - 1$, as in this case of $m + r - 1$ polynomials $\alpha_i(\theta)$ and $\beta_i(\theta)$, which are uniquely derived by solving the continuous order conditions (10), and the corresponding collocation polynomial satisfies the conditions listed in the following corollary [5].

Corollary 1. *The maximum attainable uniform order of convergence for a multivalued collocation method (2) with collocation polynomial in (5) and vector of external stages defined by (8) is $p = 2m + 1 = m + r - 1$. The corresponding collocation polynomial satisfies the following interpolation and collocation conditions:*

$$P_n(t_n) = y_n, \quad P_n(t_{n-1}) = y_{n-1}, \tag{11}$$

$$P'_n(t_n + c_i h) = f(P_n(t_n + c_i h)), \quad P'_n(t_{n-1} + c_i h) = f(P_n(t_{n-1} + c_i h)), \quad i = 1, 2, \dots, m. \tag{12}$$

2.2. Nordsieck GLM Collocation Methods

Nordsieck GLM collocation methods have been introduced in [4] and rely on the vector of external stages in the so-called Nordsieck form [37]:

$$y^{[n]} = \begin{bmatrix} y_1^{[n]} \\ y_2^{[n]} \\ \vdots \\ y_r^{[n]} \end{bmatrix} \approx \begin{bmatrix} y(t_n) \\ hy'(t_n) \\ \vdots \\ h^{r-1}y^{(r-1)}(t_n). \end{bmatrix} \tag{13}$$

With this choice for an external approximation vector, the collocation polynomial (5) is a global smooth extension of the GLM (2) with tableau (4) given by the following matrices:

$$\mathbf{A} = [\beta_j(c_i)]_{i,j=1,\dots,m} \in \mathbb{R}^{m \times m}, \quad \mathbf{U} = [\alpha_j(c_i)]_{i=1,\dots,m,j=1,\dots,r} \in \mathbb{R}^{m \times r},$$

$$\mathbf{B} = [\beta_j^{(i-1)}(1)]_{i=1,\dots,m,j=1,\dots,r} \in \mathbb{R}^{r \times m}, \quad \mathbf{V} = [\alpha_j^{(i-1)}(1)]_{i,j=1,\dots,r} \in \mathbb{R}^{r \times r},$$

Order conditions have been derived in [4], as stated in the following theorem.

Theorem 2. *A multivalued collocation method (2) with collocation polynomial in (5) and vector of external stages defined by (13) is an approximation of uniform order p to the solution of the well-posed problem approximates of the solution of (1) with uniform order p , if and only if the following conditions are satisfied:*

$$\begin{aligned} \alpha_1(\theta) &= 1 \\ \frac{\theta^\nu}{\nu!} - \alpha_{\nu+1}(\theta) - \sum_{i=1}^m \frac{c_i^{\nu-1}}{(\nu-1)!} \beta_i(\theta) &= 0, \quad \nu = 1, \dots, r-1, \\ \frac{\theta^\nu}{\nu!} - \sum_{i=1}^m \frac{c_i^{\nu-1}}{(\nu-1)!} \beta_i(\theta) &= 0, \quad \nu = r, \dots, p. \end{aligned} \tag{14}$$

Corollary 2. *The maximum attainable uniform order of convergence for a multivalued collocation method (2) with a collocation polynomial in (5) and vector of external stages defined by (13) is $m + r - 1$. The corresponding collocation polynomial satisfies the following interpolation and collocation conditions:*

$$P_n(t_n) = y_1^{[n]}, \quad P'_n(t_n) = y_2^{[n]}, \quad \dots \quad P_n^{(r-1)}(t_n) = y_{r-1}^{[n]}, \tag{15}$$

$$P'_n(t_n + c_i h) = f(P_n(t_n + c_i h)), \quad i = 1, 2, \dots, m. \tag{16}$$

2.3. Derivation of A-Stable Multivalued Collocation Methods

We describe in this section the existing procedures for the derivation of *A*-stable uniform order multivalued collocation methods. The advantages of deriving such methods lies in their efficiency in the numerical treatment of stiff problem, as they do not suffer from the order reduction phenomenon [1,2]. We recall that a numerical method is *A*-stable if its region of absolute stability includes the entire complex half-plane with a negative real part.

As we observe from Corollaries 1 and 2, the maximum attainable uniform order multivalued collocation methods with collocation polynomial in (5) and vector of external stages defined by (8) or (13) is $p = m + r - 1$. With the aim of deriving *A*-stable methods, according to the Daniel–Moore theorem [1], the order of the method cannot exceed $2m$. Therefore the following Theorem clarifies the restriction, on the number of external stages, necessary for *A*-stability. The proof can be found in [4].

Theorem 3. *An A-stable multivalued collocation method with collocation polynomial in (5) fulfills the constraint $r \leq m + 1$.*

As a consequence, two-step collocation methods of Section 2.1 cannot be *A*-stable, as for these methods $r = m + 2$, while *A*-stable Nordsieck GLM collocation methods of Section 2.2 can be derived with a suitable choice for r .

In regards to two-step collocation methods, in the paper [5], *A*-stable methods of uniform order $p = m + s, s = 1, 2, \dots, m$ have been derived by imposing not all the order conditions up to $p = 2m + 1$, but just requiring the fulfillment of the first $m + s$ order conditions in (10). This procedure corresponds to relaxing some of the interpolation/collocation conditions in (11) and (12), and the corresponding methods are called two-step almost collocation methods.

In regards to Nordsieck GLM collocation methods, in the paper [4], *A*-stable methods of uniform order $p = m + r - 1$ with $r = m + 1$ have been provided.

Regarding the computational cost of multivalued collocation methods (2)–(5), it is strongly related to the solution of the nonlinear system for the computation of the vector $Y^{[n]}$ in (2), and depends on the matrix $\mathbf{A} = [\beta_j(c_i)]_{i,j=1,\dots,m}$. Two-step almost collocation methods having lower triangular or diagonal coefficient matrix \mathbf{A} that have been derived in [24]. Regarding Nordsieck GLM collocation methods, the requirement for a structured coefficient matrix forces the relaxation of some of the interpolation/collocation conditions (15) and (16), thus leading to Nordsieck GLM almost collocation methods with $r = m + 1$, having order $p = r$ or $p = r - 1$, i.e., obtained by imposing not all the order conditions up to $p = m + r - 1$, but just requiring the fulfillment of the first r or $r - 1$ order conditions in (14).

We now provide examples of *A*-stable multivalued collocation and almost collocation methods belonging to the class described in Section 2.2. We consider the case of $m = 2$ and $r = m + 1 = 3$. The collocation polynomial assumes the form:

$$P_n(t_n + \vartheta h) = y_1^{[n]} + \alpha_2(\vartheta)y_2^{[n]} + \alpha_3(\vartheta)y_3^{[n]} + h(\beta_1(\vartheta)f(P(t_n + c_1h)) + \beta_2(\vartheta)f(P(t_n + c_2h))) \tag{17}$$

and the corresponding Butcher tableau is given by:

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

We consider the following forms for the matrix **A**:

- Full matrix [4] (GLM-F);
- Lower triangular matrix (GLM-T);
- Singly lower triangular matrix (GLM-S);
- Diagonal matrix (GLM-D).

Polynomials $\alpha_j(\vartheta)$ and $\beta_j(\vartheta)$ in (17) are constructed by imposing order conditions of Theorem 2 with $p = 4$ in the case of GLM-F and $p = 3$ in the case of GLM-T, GLM-S, and GLM-D. Figure 1 shows the region of *A*-stability in the (c_1, c_2) plane for all the classes of methods.

Examples of *A*-stable methods have the following Butcher tableau:

- GLM-F:

$$c = \begin{bmatrix} 3/2 \\ 9/5 \end{bmatrix}, \left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{cc|ccc} \frac{9}{8} & -\frac{125}{288} & 1 & \frac{233}{288} & \frac{7}{32} \\ \frac{162}{125} & -\frac{3}{10} & 1 & \frac{201}{250} & \frac{27}{125} \\ \hline \frac{14}{27} & -\frac{125}{486} & 1 & \frac{359}{486} & \frac{5}{27} \\ \frac{32}{27} & -\frac{125}{243} & 0 & \frac{80}{243} & \frac{4}{27} \\ \frac{8}{9} & 0 & 0 & -\frac{8}{9} & -\frac{1}{3} \end{array} \right].$$

- GLM-T:

$$c = \begin{bmatrix} 22/10 \\ 9/10 \end{bmatrix}, \left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{cc|ccc} \frac{11}{15} & 0 & 1 & \frac{22}{15} & \frac{121}{150} \\ -\frac{243}{1100} & \frac{81}{50} & 1 & -\frac{549}{1100} & -\frac{567}{1000} \\ \hline -\frac{103}{429} & \frac{24}{13} & 1 & -\frac{20}{33} & -\frac{19}{30} \\ -\frac{2}{13} & \frac{28}{13} & 0 & -1 & -\frac{3}{5} \\ \frac{118}{143} & -\frac{32}{13} & 0 & \frac{18}{11} & \frac{7}{5} \end{array} \right].$$

- GLM-S:

$$c = \begin{bmatrix} 22/10 \\ 9/10 \end{bmatrix}, \left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{cc|ccc} \frac{11}{15} & 0 & 1 & \frac{22}{15} & \frac{121}{150} \\ -\frac{351}{4840} & \frac{11}{15} & 1 & \frac{3473}{14520} & -\frac{21}{220} \\ \hline -\frac{335}{4719} & \frac{880}{1053} & 1 & \frac{2306}{9801} & -\frac{19}{198} \\ \frac{205}{4719} & \frac{3080}{3159} & 0 & -\frac{542}{29403} & \frac{8}{297} \\ \frac{2830}{4719} & -\frac{3520}{3159} & 0 & \frac{15130}{29403} & \frac{203}{297} \end{array} \right].$$

- GLM-D:

$$c = \begin{bmatrix} 3 \\ 29/10 \end{bmatrix}, \left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \mathbf{B} & \mathbf{V} \end{array} \right] = \left[\begin{array}{cc|ccc} 1 & 0 & 1 & 2 & \frac{3}{2} \\ 0 & \frac{29}{30} & 1 & \frac{29}{15} & \frac{841}{600} \\ \hline \frac{209}{15} & -\frac{37520}{2523} & 1 & \frac{24446}{12615} & \frac{1589}{870} \\ -\frac{62}{5} & \frac{11260}{841} & 0 & \frac{47}{4205} & -\frac{91}{145} \\ -\frac{91}{15} & \frac{5660}{841} & 0 & -\frac{8369}{12165} & -\frac{46}{145} \end{array} \right].$$

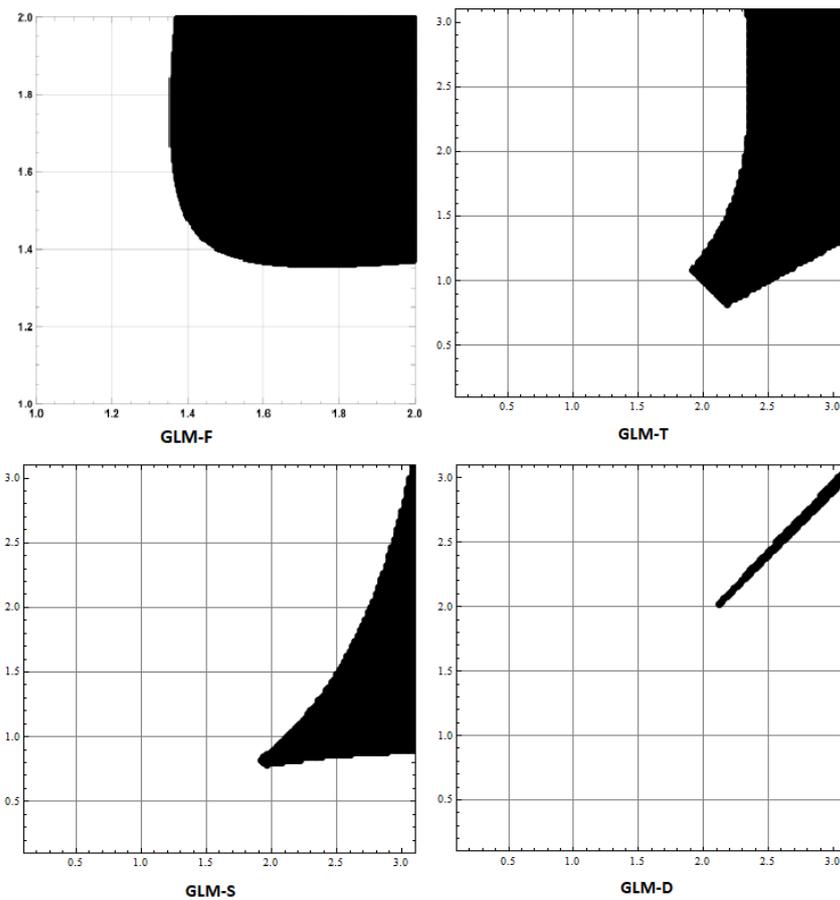


Figure 1. Regions of A-stability in the (c_1, c_2) plane.

2.4. Numerical Illustration

We now show the behavior of the methods listed in the previous section on the Prothero–Robinson problem [1,2]:

$$\begin{cases} y'(t) = \lambda(y(t) - \sin(t)) + \cos(t), & t \in [0, 10], \\ y(0) = 0, \end{cases} \tag{18}$$

which is stiff when $\lambda \ll 0$. We compare the results of the aforementioned methods with those obtained by the two-stage Gaussian Runge–Kutta (RK) method. We report in Table 1 the results obtained for $\lambda = -10^6$ in (18), by applying multivalue collocation and almost collocation methods together with the Runge–Kutta (RK) method of Gauss:

$$\begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array} \tag{19}$$

The method (19), which has order 4 and uniform order 2, therefore suffers from order reduction when applied to a stiff problem. Table 1 shows the error in the final step point for different values of the step size and the experimental order of the methods for $\lambda = -10^6$. We observe that the Runge–Kutta method exhibits order reduction, while this is not the case for multivalue collocation and almost collocation methods, having order 4 but uniform order 2, hence it suffers from order reduction on stiff problems, as is visible from

Table 1. Multivalued collocation and almost collocation methods, instead, keep their order of convergence.

Table 1. Absolute errors in the final step point and experimental orders of convergence for problem (18) with $\lambda = -10^6$.

h	GLM-F Error	p	GLM-T Error	p	GLM-S Error	p	GLM-D Error	p	RK Error	p
1/10	2.41×10^{-8}		1.51×10^{-7}		1.51×10^{-7}		4.88×10^{-5}		1.52×10^{-4}	
1/20	7.50×10^{-10}	5.01	9.21×10^{-9}	4.03	9.21×10^{-9}	4.03	3.04×10^{-6}	4.01	3.84×10^{-5}	1.98
1/40	2.21×10^{-11}	5.08	5.69×10^{-10}	4.02	5.70×10^{-10}	4.01	1.89×10^{-7}	4.01	9.99×10^{-6}	1.94
1/80	7.06×10^{-13}	4.97	3.45×10^{-11}	4.04	3.58×10^{-11}	3.99	1.18×10^{-8}	4.00	2.78×10^{-6}	1.85

3. Multivalued Mixed Collocation Methods

In this Section we describe the derivation of Nordsieck GLM mixed collocation methods of the form (2)–(5), with the vector of external stages in Nordsieck form (13). The idea is, instead of considering a basis of polynomials $\{\alpha_i(\theta), \beta_j(\theta), i = 1, \dots, r, j = 1, \dots, m\}$, to consider a basis constituted by a combination of trigonometric and polynomial functions. Such methods are useful for problems of the form (1) for which the exact solution is oscillatory with a known frequency of oscillation ω .

As a consequence of Theorem 2, the polynomials $\alpha_i(\theta)$ and $\beta_j(\theta)$, associated to Nordsieck GLM collocation methods of uniform order $p = m + r - 1$, have a degree of at most $m + r - 1$. Therefore, they can be written in the form:

$$\alpha_1(\theta) = 1 \quad \alpha_{i+1}(\theta) = \sum_{j=1}^{m+r-1} \frac{\bar{\mu}_{i,j-1}}{j} \theta^j, \quad i = 1, \dots, r - 1, \quad (20)$$

$$\beta_i(\theta) = \sum_{j=1}^{m+r-1} \frac{\mu_{i,j-1}}{j} \theta^j, \quad i = 1, \dots, m. \quad (21)$$

The idea of Nordsieck GLM mixed collocation methods introduced in [35] relies on considering new basis functions:

$$\{\alpha_i^T(\theta, z), \beta_j^T(\theta, z), i = 1, \dots, r, j = 1, \dots, m\},$$

which depend also on the frequency of oscillation of the problem, i.e., depending on $z = \omega h$, of the form:

$$\alpha_1^T(\theta, z) = 1, \quad (22)$$

$$\alpha_{i+1}^T(\theta, z) = \frac{\bar{a}_i}{z} \sin(z\theta) - \frac{\bar{b}_i}{z} \cos(z\theta) + \frac{\bar{b}_i}{z} + \sum_{j=1}^{m+r-3} \frac{\bar{\gamma}_{i,j-1}}{j} \theta^j \quad i = 1, \dots, r - 1, \quad (23)$$

$$\beta_i^T(\theta, z) = \frac{a_i}{z} \sin(z\theta) - \frac{b_i}{z} \cos(z\theta) + \frac{b_i}{z} + \sum_{j=1}^{m+r-3} \frac{\gamma_{i,j-1}}{j} \theta^j \quad i = 1, \dots, m. \quad (24)$$

The next theorem shows the expressions of coefficients $a_i, b_i, \gamma_{i,j}$ in (23) and $\bar{a}_i, \bar{b}_i, \bar{\gamma}_{i,j}$ in (24) in order to obtain the maximum attainable uniform order $p = m + r - 1$. The proof can be found in [35].

Theorem 4. A multivalued mixed collocation method (2)–(5), with vector of external stages defined by (13) and functional basis $\{\alpha_i(\theta), \beta_j(\theta), i = 1, \dots, r, j = 1, \dots, m\}$ defined in (22)–(24), has order $p = m + r - 1$ if:

$$a_i = \frac{\det M_{i,1}}{\det M}, \quad b_i = \frac{\det M_{i,2}}{\det M}, \quad i = 1, \dots, m, \quad (25)$$

$$\gamma_{ij} = \begin{cases} (-1)^{\frac{j}{2}+1} a_i \frac{z^j}{j!} & j \text{ is even,} \\ (-1)^{\frac{j+1}{2}} b_i \frac{z^j}{j!} & j \text{ is odd,} \\ \frac{\det M_{i,j-r+4}}{\det M} & \end{cases} \quad \begin{matrix} j = 0, \dots, r-2, \\ \\ j = r-1, \dots, m+r-4, \end{matrix} \quad , i = 1, \dots, m, \quad (26)$$

$$\bar{a}_i = \frac{\sum_{k=1}^m (-1)^{k+1} \frac{c_k^{i-1}}{(i-1)!} \det M_{k,1}}{\det M}, \quad \bar{b}_i = \frac{\sum_{k=1}^m (-1)^k \frac{c_k^{i-1}}{(i-1)!} \det M_{k,2}}{\det M}, \quad i = 1, \dots, r-1, \quad (27)$$

$$\bar{\gamma}_{ij} = \begin{cases} (-1)^{\frac{j}{2}+1} \bar{a}_i \frac{z^j + \delta_{i,j+1}}{j!} & j \text{ is even,} \\ (-1)^{\frac{j+1}{2}} \bar{b}_i \frac{z^j + \delta_{i,j+1}}{j!} & j \text{ is odd,} \\ \frac{\sum_{k=1}^m (-1)^{k+j-r+1} \frac{c_k^{i-1}}{(i-1)!} \det M_{k,j-r+4}}{\det M} & \end{cases} \quad \begin{matrix} j = 0, \dots, r-2, \\ \\ j = r-1, \dots, m+r-4, \end{matrix} \quad , i = 1, \dots, r-1, \quad (28)$$

where M is a square non singular matrix of order m given by:

$$M = \begin{pmatrix} \cos(zc_1) - \sum_{k=0}^{r_1} (-1)^k \frac{(zc_1)^{2k}}{(2k)!} & \sin(zc_1) - \sum_{k=0}^{r_2} (-1)^k \frac{(zc_1)^{2k+1}}{(2k+1)!} & c_1^{r-1} & c_1^r & \dots & c_1^{m+r-4} \\ \cos(zc_2) - \sum_{k=0}^{r_1} (-1)^k \frac{(zc_2)^{2k}}{(2k)!} & \sin(zc_2) - \sum_{k=0}^{r_2} (-1)^k \frac{(zc_2)^{2k+1}}{(2k+1)!} & c_2^{r-1} & c_2^r & \dots & c_2^{m+r-4} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cos(zc_m) - \sum_{k=0}^{r_1} (-1)^k \frac{(zc_m)^{2k}}{(2k)!} & \sin(zc_m) - \sum_{k=0}^{r_2} (-1)^k \frac{(zc_m)^{2k+1}}{(2k+1)!} & c_m^{r-1} & c_m^r & \dots & c_m^{m+r-4} \end{pmatrix},$$

$M_{i,j}$ is the submatrix obtained by deleting the i -th row and j -th column from matrix M , c_1, \dots, c_m are the collocation points, δ_{ij} is the usual Kronecker delta, and:

$$r_1 = \begin{cases} \frac{r-2}{2} & r \text{ is even,} \\ \frac{r-3}{2} & r \text{ is odd,} \end{cases} \quad r_2 = \begin{cases} \frac{r-2}{2} - 1 & r \text{ is even,} \\ \frac{r-3}{2} & r \text{ is odd.} \end{cases}$$

In order to show the performance of Nordsieck GLM mixed collocation methods, we show the results obtained on the following test problems:

- Problem 1:

$$\begin{cases} y'(t) = -(y(t) - \sin(\omega t)) + \omega \cos(\omega t), & t \in [0, 10] \\ y(0) = 0, \end{cases} \quad (29)$$

whose solution is $y(t) = \sin(\omega t)$, so it is a function belonging to the basis.

- Problem 2:

$$\begin{cases} y'(t) = -(y(t) - \sin(\omega t + t)) + (\omega + 1) \cos(\omega t + t), & t \in [0, 10] \\ y(0) = 0, \end{cases} \quad (30)$$

whose solution is $y(t) = \sin(\omega t + t) = \sin \omega t \cos t + \cos \omega t \sin t$, so it is a combination of the basic functions $\sin \omega t$ and $\cos \omega t$.

We put $m = 2$ and $r = 3$ and $c_1 = 3/2, c_2 = 9/5$ and we denote by MGLM-F, the corresponding Nordsieck GLM mixed collocation method. In Table 2, we consider for a comparison, the GLM-F method of Section 2.3. The table clearly shows the advantage of mixed collocation versus polynomial collocation in the case of the oscillatory solution.

Table 2. Absolute errors (in the final step point) and effective orders of convergence. Absolute errors in the final step point and experimental orders of convergence with $\omega = 100$.

h	GLM-F on Problem (29) Error	MGLM-F on Problem (29) Error	GLM-F on Problem (30) Error	p	MGLM-F on Problem (30) Error	p
1/40	0.2764	1.4818×10^{-12}	0.3626		0.0133	
1/80	0.0326	8.4277×10^{-13}	0.0436	3.0560	9.5762×10^{-4}	3.7958
1/160	0.0024	1.2212×10^{-15}	0.0031	3.8140	6.1966×10^{-5}	3.9499
1/320	1.5567×10^{-4}	8.9595×10^{-14}	1.9729×10^{-4}	3.9739	3.9064×10^{-6}	3.9876
1/640	9.8558×10^{-6}	1.4988×10^{-14}	1.2403×10^{-5}	3.9916	2.4468×10^{-7}	3.9969

4. Multivalued Spline Collocation Methods for FDEs

In this section, we review multivalued spline collocation methods [18,20,54], applied to the IVP problem of type:

$$\begin{cases} D^\alpha y(t) = f(t, y(t)), & t \in [0, b], \\ y^{(i)}(0) = \gamma_i, & i = 0, \dots, n - 1, \end{cases} \tag{31}$$

where $n - 1 < \alpha < n, n \in \mathbb{N}, \gamma_i \in \mathbb{R}, f : [0, b] \times \mathbb{R} \rightarrow \mathbb{R}$. Here we consider the Caputo fractional derivative [58–60]:

$$D^\alpha y(t) = \frac{1}{\Gamma(n - \alpha)} \int_0^t \frac{y^{(n)}(s)}{(t - s)^{\alpha + 1 - n}} ds.$$

The convergence analysis of spline collocation methods is carried out in the functional space $C^{q,\nu}(0, T]$, defined as follows [15].

Let $q \in \mathbb{N}$ and $\nu \in (-\infty, 1)$, then $y : [0, T] \rightarrow \mathbb{R}$ belongs to the space $C^{q,\nu}(0, T]$ if it is q times continuously differentiable in $(0, T]$, and:

$$|y^{(i)}(t)| \leq c \begin{cases} 1 & \text{if } i < 1 - \nu, \\ 1 + |\log t| & \text{if } i = 1 - \nu, \\ t^{1-\nu-i} & \text{if } i > 1 - \nu, \end{cases} \quad t \in (0, T], i = 1, \dots, q.$$

Sufficient conditions for obtaining a solution in the space $C^{q,\nu}(0, T]$ are provided by the following theorem.

Theorem 5 ([30]). Let $f \in C([0, T] \times \mathbb{R})$, q times continuously differentiable in $(0, T] \times \mathbb{R}$, and $\exists \nu \in [1 - \alpha, 1)$ such that:

$$\left| \frac{\partial^{i+j}}{\partial t^i \partial y^j} f(t, y) \right| \leq \phi(|y|) \begin{cases} 1 & \text{if } i < 1 - \nu \\ 1 + |\log t| & \text{if } i = 1 - \nu \\ t^{1-\nu-i} & \text{if } i > 1 - \nu \end{cases}, (t, y) \in (0, T] \times \mathbb{R},$$

$\forall i, j \in \mathbb{N}$ with $i + j \leq q$. In addition, for $\alpha \in (0, 1)$ assume that:

$$\left| \frac{\partial^{i+j}}{\partial t^i \partial y^j} [f(t, y_1) - f(t, y_2)] \right| \leq \phi(\max\{|y_1|, |y_2|\}) |y_1 - y_2| \begin{cases} 1 & \text{if } i = 0 \\ t^{1-\nu-i} & \text{if } i > 0 \end{cases},$$

$(t, y_i) \in (0, T] \times \mathbb{R}, i = 1, 2$. The function $\phi : [0, \infty) \rightarrow \mathbb{R}$ is assumed to be monotonically increasing. Let the fractional IVP (31) have a solution $y \in C[0, T]$ with $D^\alpha y \in C[0, T]$. Then $y \in C^{q,\nu}(0, T]$ and $D^\alpha y \in C^{q,\nu}(0, T]$.

By setting $z = D^\alpha y$, we have:

$$y = J^\alpha z + Q, \tag{32}$$

with,

$$(J^\alpha z)(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} z(s) ds, \quad t > 0, \tag{33}$$

$$Q(t) = \sum_{i=0}^{[\alpha]-1} \frac{\gamma_i}{i!} t^i, \tag{34}$$

$[\alpha]$ being the smallest integer not less than α . With this position, we may rewrite the IVP (31) as a nonlinear equation:

$$z = f(t, J^\alpha z + Q). \tag{35}$$

Once (35) is solved, y can be computed by (32).

4.1. One-Step Collocation Methods for FDEs

Let us introduce a graded mesh I_N on $[0, T]$ with grading exponent $r \geq 1$:

$$t_j = b \left(\frac{j}{N} \right)^r, \tag{36}$$

and collocation parameters $0 \leq \eta_1 < \dots < \eta_m \leq 1$. Let,

$$S_k^{(-1)}(I_N) = \{v : v|_{[t_{j-1}, t_j]} \in \Pi_k, j = 1, \dots, N\}. \tag{37}$$

The one step collocation method approximates the solution z of (35) by a function $v \in S_{m-1}^{(-1)}(I_N)$. The collocation solution v is computed by imposing these collocation conditions, for $j = 1, \dots, N$:

$$v_j(t_{jk}) = f(t_{jk}, (J^\alpha v)(t_{jk}) + Q(t_{jk})), \quad k = 1, \dots, m. \tag{38}$$

where $v_j := v|_{[t_{j-1}, t_j]}$. Then, the approximate solution of (31) is the function y_N , defined as:

$$y_N = J^\alpha v + Q. \tag{39}$$

Collocation conditions (38) give rise to the nonlinear system in the unknowns $z_{jk} := v_j(t_{jk})$:

$$z_{jk} = f \left(t_{jk}, \sum_{\mu=1}^m z_{j\mu} (J^\alpha \varphi_{j,\mu})(t_{jk}) + \sum_{\lambda=1}^{j-1} \sum_{\mu=1}^m z_{\lambda\mu} (J^\alpha \varphi_{\lambda,\mu})(t_{jk}) + Q(t_{jk}) \right), \quad k = 1, \dots, m,$$

where $\varphi_{\lambda,\mu}$ is equal to the μ -th Lagrange fundamental polynomial corresponding to the nodes $t_{\lambda 1}, \dots, t_{\lambda m}$ in $[t_{\lambda-1}, t_\lambda]$, and it is null outside this interval.

The error is analyzed in the following theorem, where this quantity is used:

$$E_N(p, \nu, r) = \begin{cases} N^{-r(1-\nu)} & \text{if } 1 \leq r \leq \frac{p}{1-\nu} \\ N^{-p}(1 + \log N) & \text{if } r = \frac{p}{1-\nu} = 1 \\ N^{-p} & \text{if } r = \frac{p}{1-\nu} > 1 \text{ or } r > \frac{p}{1-\nu}. \end{cases} \tag{40}$$

Theorem 6 ([30], [Th. 4.1]). *Let the IVP (31) have a solution $y \in C[0, b]$, with $D^\alpha y \in C[0, b]$ and let $f \in C([0, b] \times \mathbb{R})$ such that its derivatives $\frac{\partial}{\partial t} f(t, y)$ and: $\frac{\partial^2}{\partial t^2} f(t, y)$ are continuous in $(0, b] \times \mathbb{R}$ and*

$$\left| \frac{\partial^j}{\partial y^j} f(t, y) \right| \leq \psi(|y|), \quad (t, x) \in (0, b] \times \mathbb{R}, j = 0, 1, 2.$$

$\psi : [0, \infty) \rightarrow \mathbb{R}$ is a monotonically increasing function.

Then there exist $N_0 \in \mathbb{N}$ and $\delta_0 > 0$ such that, for all $N \geq N_0$, the one-step collocation method possesses a unique solution $v \in S_{m-1}^{(-1)}(I_N)$ in the ball $\|u - z\|_\infty \leq \delta_0$, where $z = D^\alpha y \in C[0, b]$. If, in addition, the assumptions of Theorem 5 with $q := m$ and $v \in [1 - \alpha, 1)$ are fulfilled, then for all $N \geq N_0$, the following error estimate holds:

$$\|y_N - y\|_\infty \leq cE_N(m, v, r),$$

with y_N given by Formula (39). Here c is a constant not depending on N , and E_N is defined by (40).

4.2. Two-Step Collocation Methods for FDEs

Given the graded mesh I_N defined in (36) and collocation parameters $0 \leq \eta_1 < \dots < \eta_m \leq 1$, with $(\eta_1, \eta_m) \neq (0, 1)$, the two-step collocation method approximates the solution z of (35) by a function $v \in S_{2m-1}^{(-1)}(I_N)$. By defining the polynomial $v_j = v|_{[t_{j-1}, t_j]}$, we impose these collocation and interpolation conditions, for $j = 2, \dots, N$:

$$v_j(t_{jk}) = f(t_{jk}, (J^\alpha v)(t_{jk}) + Q(t_{jk})), \quad k = 1, \dots, m \tag{41}$$

$$v_j(t_{j-1,k}) = v_{j-1}(t_{j-1,k}), \quad k = 1, \dots, m \tag{42}$$

The collocation solution $v(t)$ can be expressed as:

$$v(t) = v_1(t) + \sum_{\lambda=2}^N \left(\sum_{k=1}^m z_{\lambda k} L_{\lambda, m+k}(t) + \sum_{k=1}^m z_{\lambda-1, k} L_{\lambda k}(t) \right), \quad t \in [0, T], \tag{43}$$

where v_1 is obtained by a suitable starting procedure (cfr. [20]); $L_{\lambda, \mu} = L_\mu$ in $[t_{\lambda-1}, t_\lambda]$ and it is null outside. L_μ is the μ -th Lagrange fundamental polynomial corresponding to the nodes $\{t_{j-1, k}, t_{j, k} \mid k = 1, \dots, m\}$. The coefficients $z_{\lambda \mu}$ are the solution of the nonlinear system:

$$z_{jk} = f(t_{jk}, (J^\alpha v)(t_{jk}) + Q(t_{jk})), \quad k = 1, \dots, m.$$

A more explicit formulation of the above system is:

$$z_{jk} = f \left(t_{jk}, (J^\alpha v_1)(t_{jk}) + \sum_{\mu=1}^m z_{j\mu} (J^\alpha L_{j, m+\mu})(t_{jk}) + \sum_{\lambda=2}^{j-1} \sum_{\mu=1}^m z_{\lambda \mu} (J^\alpha L_{\lambda, m+\mu})(t_{jk}) + \sum_{\mu=1}^m z_{j-1, \mu} (J^\alpha L_{j\mu})(t_{jk}) + \sum_{\lambda=2}^{j-1} \sum_{\mu=1}^m z_{\lambda-1, \mu} (J^\alpha L_{\lambda \mu})(t_{jk}) + Q(t_{jk}) \right), \tag{44}$$

$k = 1, \dots, m$. Although a number of fractional integrals must be computed, they may be analytically evaluated, thus no further approximation is needed.

The main converge result is provided by the following theorem:

Theorem 7 ([20], [Th. 4.5]). *Let hypothesis HP 1 of Theorem 6 hold. Then there exist $N_0 \in \mathbb{N}$ and $\delta_0 > 0$ such that, for all $N \geq N_0$, the two-step collocation method possesses a unique solution $v \in S_{2m-1}^{(-1)}(I_N)$ in the ball $\|u - z\|_\infty \leq \delta_0$, where $z = D^\alpha y \in C[0, T]$. If, in addition, the assumptions of Theorem 5 with $q := 2m$ and $v \in [1 - \alpha, 1)$ are satisfied, then for all $N \geq N_0$, the error is bounded as follows:*

$$\|y_N - y\|_\infty \leq cE_N(2m, v, r),$$

with y_N defined in (39). Here, the value of the constant c does not depend on N , and E_N is defined in (40).

It is evident that a suitable choice of the grading exponent r is the basic step to obtain a high accuracy. The best choice of r grows with m , i.e., with the number of collocation abscissae and also depends on the degree of smoothness of the analytical solution.

By comparing one- and two-step collocation methods, we observe that they have the same computational cost, since they both require the solution of a nonlinear system of dimension m , nevertheless, the error of the two-step method decreases as $O(N^{-2m})$, while the error of the one-step method decreases as $O(N^{-m})$ (for both methods we considered the best case).

We provide a numerical illustration on the following test equation, taken from [61].

$$D^\alpha y(t) = \frac{40320}{\Gamma(9-\alpha)} t^{8-\alpha} - 3 \frac{\Gamma(5+\frac{\alpha}{2})}{\Gamma(5-\frac{\alpha}{2})} t^{4-\frac{\alpha}{2}} + \left(\frac{3}{2} t^{\frac{\alpha}{2}} - t^4\right)^3 t \in [0, 1],$$

$$+ \frac{9}{4} \Gamma(\alpha+1) - (y(t))^{\frac{3}{2}},$$

$$y(0) = 0,$$

$\alpha = 1/2$. The exact solution is $y = t^8 - 3t^{4+\alpha/2} + \frac{9}{4}t^\alpha$. The hypotheses of Theorem 5 are satisfied by $\nu = 0.5$ and any $q \in \mathbb{N}$. In Figure 2, we plot the work-precision diagram obtained by one- and two-step collocation methods, with collocation parameters equally spaced in $[0, 1]$ with $\eta_0 \neq 0$ and $\eta_m \neq 1$; with $r = \frac{m}{1-\nu}$ for the one-step methods and $r = \frac{2m}{1-\nu}$ for the two-step methods. We observe that multivalue collocation obtain a definite improvement of one-step collocation methods, except for low accuracy requests.

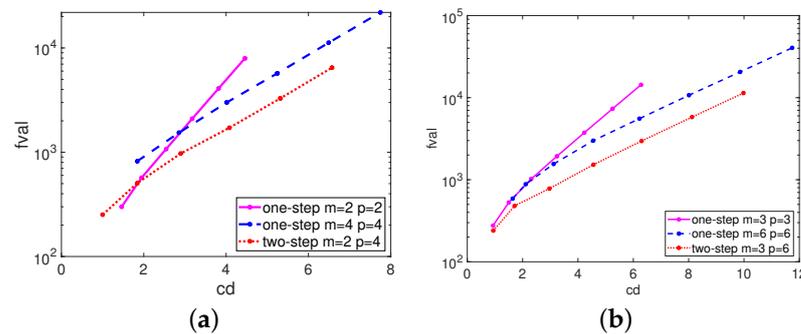


Figure 2. Work-precision diagrams for one- and two-step collocation methods for FDEs, cd is the number of correct digits, and $fval$ is the number of function evaluations. (a) One-step methods with $m = 2$ and $m = 4$, two-step methods with $m = 2$; (b) one-step methods with $m = 3$ and $m = 6$, two step methods with $m = 3$.

5. Conclusions

We presented a concise selection of our recent results on collocation methods for ODEs and FDE. This technique has exhibited a wide range of benefits in terms of accuracy and efficiency. Moreover, the choice of collocation basis makes the numerics more adapted to the problem, with meaningful improvements when qualitative behaviors of the solution are merged in the numerical scheme. Adapted functional basis are relevant, for instance, in the case of oscillatory problems [62–65]. Further developments of this research will be oriented to the establishment of a theory of collocation methods for stochastic problems (see, for instance, refs. [51,66–71] and references therein).

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Abbreviations

The following abbreviations are used in this manuscript:

FDEs	Fractional Differential Equation
GLM	General Linear Method
IVP	Initial Value Problem
ODE	Ordinary Differential Equation
RK	Runge–Kutta

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