Practical Construction of Two-Step Collocation Runge-Kutta Methods for Ordinary Differential Equations

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It is the purpose of this paper to analyse a new class of two-step collocation methods for the numerical solution of ordinary differential equations (ODEs), possessing higher order of convergence than classical one step collocation methods and A-stability, without any increase of the computational cost.

These methods seem to be particularly promising for practical applications, e.g. efficient implementation, resolution of ODEs based problems belonging to models of evolutionary real life phenomena.

Keywords: Ordinary differential equations; Collocation methods; Two-step Runge–Kutta methods; A-stability.

1. Introduction

We are concerned with the numerical solution of initial value problems based on ordinary differential equations of the type

$$\begin{cases} y'(x) = f(x, y(x)), & x \in I = [x_0, X] \\ y(x_0) = y_0, \end{cases} \tag{1}$$

with $f : I \times \Omega \subset \mathbb{R}^d \to \mathbb{R}^d$ smooth enough to guarantee that the problem (1) is well-posed.

The methods we aim to derive belong to a special family of two-step

Runge–Kutta methods (TSRK), of the type

$$Y_j^{[n]} = y_n + h\sum_{i=1}^{m}[a_{ij}f(Y_i^{[n-1]}) + b_{ij}f(Y_i^{[n]})], \tag{2}$$

$$y_{n+1} = y_n + h\sum_{j=1}^{m}[v_j f(Y_j^{[n-1]}) + w_j f(Y_j^{[n]})], \tag{3}$$

with $j = 1, 2, ..., m$, depending on the stage derivatives at two consecutive step points. As pointed out in [12], methods of this type are interesting because it is possible to introduce more parameters to play with in order to obtain higher order and better stability properties than classical Runge–Kutta methods, without any increase in the computational cost: in fact, advancing from x_n to x_{n+1}, the stage derivatives $f(Y_j^{[n-1]})$, $j = 1, 2, ..., m$, have already been computed. Starting values are generally determined using a classical Runge–Kutta method of the same order.

In this paper we consider an extension of algebraic multistep collocation technique (see [9,10,15)], in order to obtain continuous, high effective order, highly stable methods of the type (2)-(3). It seems interesting and promising to look at TSRK methods of the type (2)-(3), because of what follows. In [5,6] we have extended this idea to a more general class of TSRK methods, introduced by Jackiewicz and Tracogna in [12], of the type

$$Y_j^{[n]} = u_j y_{n-1} + (1-u_j)y_n + h\sum_{i=1}^{m}[a_{ij}f(Y_i^{[n-1]}) + b_{ij}f(Y_i^{[n]})], \tag{4}$$

$$y_{n+1} = \theta y_{n-1} + (1-\theta)y_n + h\sum_{j=1}^{m}[v_j f(Y_j^{[n-1]}) + w_j f(Y_j^{[n]})], \tag{5}$$

deriving formulas of order $2m+1$, but having only bounded stability regions. In order to gain better stability properties, we have considered in [7] possible ways to relax the requirements imposed in [5,6], with a corresponding improvement in the stability (in fact we have obtained A-stable and L-stable formulas), but obtaining lower order of convergence. Therefore, in order to have a good balance between effective order and high stability, it is convenient to study methods of the type (2)-(3): Jackiewicz and Tracogna themselves derive in [12] examples of methods (4)-(5) with $\theta = 0$, $u_j = 0$, $j = 1, 2, ..., m$, emphasizing on the corresponding advantage in terms of stability and also simplifying the system of order conditions (see [12]).

Collocation methods of the type (2)-(3) are also very interesting in view of an efficient implementation (e.g. variable stepsize, variable order implementation, also in a parallel environment), as it has been showed, although outside collocation, in [2–4,13,20,22,23].

The paper is organized as follows: in Section 2 we discuss on the construction of two-step algebraic collocation methods of the type (2)-(3) and derive continuous order conditions for these methods in Section 3. Section 4 is focused on the linear stability analysis: in particular, we will discuss on the existence of A-stable methods within the class of collocation based methods (2)-(3). Examples of methods are provided in Section 5.

2. General two–step collocation methods

The classical collocation technique consists in the derivation of an algebraic polynomial $P(x_n + sh)$, satisfying suitable interpolation and collocation conditions: in particular, this polynomial exactly solves the equation (1) at some points. In order to derive collocation based methods of the type (2)-(3), we impose the following set of conditions:

$$P(x_n) = y_n, \tag{6}$$

$$P'(x_{n-1} + c_i h) = f(x_{n-1} + c_i h, P(x_{n-1} + c_i h)), \quad i = 1, 2, ..., m, \tag{7}$$

$$P'(x_n + c_i h) = f(x_n + c_i h, P(x_n + c_i h)), \quad i = 1, 2, ..., m. \tag{8}$$

Equation (6) is an interpolation condition, while conditions (7)-(8) form a set of $2m$ collocation conditions with respect to two consecutive step points. Introducing the dimensionless coordinate $t = \frac{x-x_n}{h}$, it is convenient to express the collocation polynomial in the following form

$$P(x_n + th) = \varphi(t)y_n + h\sum_{j=1}^{m}\big[\chi_j(t)P'(x_{n-1} + c_j h) + \psi_j(t)P'(x_n + c_j h)\big],$$

i.e. as linear combination of $2m + 1$ basis polynomials

$$\{\varphi(t),\ \chi_j(t),\ \psi_j(t), \quad j = 1, 2, ..., m\}.$$

In order to determine this $2m+1$ unknown basis functions, we apply the set of conditions (6)-(7)-(8), i.e.

$$\phi(0) = 1, \qquad \chi_i(0) = 0, \qquad \psi_i(0) = 0, \tag{9}$$

$$\phi'(c_i - 1) = 0,\, \chi'_j(c_i - 1) = \delta_{ij},\, \psi'_j(c_i - 1) = 0, \tag{10}$$

$$\phi'(c_i) = 0, \qquad \chi'_j(c_i) = 0, \qquad \psi'_j(c_i) = \delta_{ij}, \tag{11}$$

for $i, j = 1, 2, \ldots, m$, where δ_{ij} is the usual Kronecker delta. Therefore, each basis polynomial is subject to $2m+1$ conditions, which uniquely define polynomials of degree at most $2m$. Therefore, the polynomial $P(x_n + th)$ is uniquely determined as linear combination of polynomials of degree at most $2m$ and, correspondingly, we compute $y_{n+1} = P(x_n + h)$. We omit for brevity the details of the resolution of the systems of equations arising from (9)-(10)-(11), which can be inferred, with simple modifications, from [5,6]. The expressions of the basis polynomials are available through e-mail from the authors.

We conclude this section with the following result of characterization of TSRK collocation methods.

Theorem 2.1. *The method defined by (9)-(10)-(11) is equivalent to a TSRK method (2)-(3), with*

$$\begin{array}{l} v_j = \chi_j(1), \quad w_j = \psi_j(1), \\ a_{ij} = \chi_j(c_i),\, b_{ij} = \psi_j(c_i), \end{array}$$

for $i,\ j, = 1,\ \ldots,\ m.$

Proof. The proof follows along the line of Theorem 1 on p. 739 in [6]. □

3. Order conditions.

In this section we derive continuous order conditions for collocation methods having the following form

$$\begin{cases} P(x_n + sh) = \varphi(s) y_n + \\ \qquad\qquad +h \sum_{j=1}^{m} \left[\chi_j(s) P'(x_{n-1} + c_j h) + \psi_j(s) P'(x_n + c_j h) \right], \\ y_{n+1} = P(x_{n+1}), \end{cases} \tag{12}$$

which are the continuous extensions of methods (2)-(3). We assume that $P(x_n + sh)$ is an uniform approximation to $y(x_n + sh)$, $s \in [0, 1]$, of order p.

As a consequence, the stage values $P(x_n + c_j h)$ have stage order $q = p$. We now introduce the local discretization error $\xi(x_n + sh)$, which is defined as the residuum obtained by replacing $P(x_n + sh)$ by $y(x_n + sh)$, $P(x_n + c_j h)$ by $y(x_n + c_j h)$, $j = 1, 2, \ldots, m$, y_{n-1} by $y(x_{n-1})$ and y_n by $y(x_n)$, where $y(x)$ is the exact solution. This leads to

$$\begin{aligned}\xi(x_n + sh) &= y(x_n + sh) - \varphi(s)y(x_n) \\ &\quad - h\textstyle\sum_{j=1}^{m}\Big(\chi_j(s)y'(x_n + (c_j - 1)h) + \psi_j(s)y'(x_n + c_j h)\Big),\end{aligned} \tag{13}$$

$s \in [0, 1]$, $n = 1, 2, \ldots, N-1$. We have the following theorem.

Theorem 3.1. *Assume that the function $f(y)$ is sufficiently smooth. Then the method (12) has uniform order p if the following conditions are satisfied*

$$\begin{cases}\varphi_1(s) = 1, \\ \sum_{j=1}^{m}\left(\chi_j(s)\frac{(c_j-1)^{k-1}}{(k-1)!} + \psi_j(s)\frac{c_j^{k-1}}{(k-1)!}\right) = \frac{s^k}{k!},\end{cases} \tag{14}$$

$s \in [0, 1]$, $k = 1, 2, \ldots, p$.
Moreover, the local discretization error (13) takes the form

$$\xi(x_n + sh) = h^{p+1}C_p(s)y^{(p+1)}(x_n) + O(h^{p+2}), \tag{15}$$

as $h \to 0$, where the error function $C_p(s)$ is defined by

$$C_p(s) = \frac{s^{p+1}}{(p+1)!} - \sum_{j=1}^{m}\left(\chi_j(s)\frac{(c_j - 1)^p}{p!} + \psi_j(s)\frac{c_j^p}{p!}\right). \tag{16}$$

Proof. We expand $y(x_n + sh)$, $y'(x_n + (c_j - 1)h)$ and $y'(n_n + c_j h)$ into Taylor series around the point x_n and next substitute them in 13. Collecting the terms appearing with the same powers of h, we obtain

$$\begin{aligned}\xi(x_n + sh) &= \Big(1 - \varphi_1(s)\Big)y(x_n) + \sum_{k=1}^{p+1}\frac{s^k}{k!}h^k y^{(k)}(t_n) \\ &\quad - \sum_{k=1}^{p+1}\sum_{j=1}^{m}\left(\chi_j(s)\frac{(c_j - 1)^{k-1}}{(k-1)!} + \psi_j(s)\frac{c_j^{k-1}}{(k-1)!}\right)h^k y^{(k)}(t_n) \\ &\quad + O(h^{p+2}).\end{aligned}$$

Equating to zero the terms of order k, $k = 0, 1, \ldots, p$, we obtain order conditions (14). Comparing the terms of order $p + 1$ we obtain (15) with error function $C_p(s)$ defined by (16). □

As a consequence of the above result, we can infer the following

Theorem 3.2. *Each method within the class (12) has order* $2m$*, for any value of* $s \in (0,1]$.

Proof. The proof results as an extension of Theorems (2.3) and (2.4) in [7]. $\square$

According to Theorem 3.2, each collocation method within the class (12) has uniform order $2m$, i.e. the order of convergence is $2m$ in any point of the integration interval. This aspect is very interesting in the applications, in particular for an accurate and efficient variable stepsize - variable order implementation of stiff systems, because having uniform order of convergence avoids the order reduction phenomenon (see [1]). Classical collocation based Runge–Kutta methods suffer of order reduction, because they have low stage order: for example, Gaussian Runge–Kutta methods have order $2m$ in the external stages, but only m in the internal ones.

4. Linear Stability Analysis

In order to investigate the linear stability properties of the methods, we recast the methods (2)-(3) as general linear methods (see [1,11]) of the form

$$\left[\begin{array}{c} Y^{[n]} \\ \hline y_{n+1} \\ hf(Y^{[n]}) \end{array}\right] = \left[\begin{array}{c|cc} A & e & B \\ \hline v^T & 1 & w^T \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} hf(Y^{[n]}) \\ \hline y_n \\ hf(Y^{[n-1]}) \end{array}\right], \tag{17}$$

where $\mathbf{I}$ is the identity matrix of dimension m and $\mathbf{0}$ is the zero matrix or vector of appropriate dimensions. The Butcher array of these methods is

$$\left[\begin{array}{c|c} \mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V} \end{array}\right] = \left[\begin{array}{c|cc} A & e & B \\ \hline v^T & 1 & w^T \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \end{array}\right]. \tag{18}$$

The corresponding stability (or amplification) matrix $M(z)$ takes the form (see [1,11])

$$M(z) = \mathbf{V} + z\mathbf{B}(I - z\mathbf{A})^{-1}\mathbf{U} \in \mathbb{R}^{(m+1)\times(m+1)} \in \mathbb{R}^{(m+1)\times(m+1)}. \tag{19}$$

We next consider the stability function of the method, it is

$$p(\omega, z) = \det\Big(\omega I - M(z)\Big), \tag{20}$$

where I is the identity matrix of order $m+1$. We investigate the conditions to impose on the collocation abscissas $c_1, \ldots, c_m$ in order to obtain A-stable methods, i.e. all the roots $\omega_1, \ldots, \omega_{m+1}$ of (20) lie in the unit circle for all $z \in \mathbb{C}$ such that $\mathrm{Re}(z) \leq 0$. The investigation, carried out using the Schur criterion (see [21]), has produced the following results for $m = 1$ and $m = 2$.

Theorem 4.1. *A-stability for $m = 1$ Any one-stage collocation based TSRK method of the type (12) is A-stable if and only if $c_1 > 1$.*

Figure 1 shows the A-stability region in the parameter space $(c1, c2)$ for collocation methods (12) with $m = 2$ and order 4.

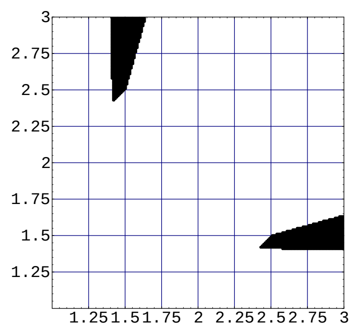

Fig. 1. Region of A-stability in the $(c1, c2)$-plane for two-step methods (12) with $m = 2$ and order 4.

5. Examples of methods

We now provide some examples of two step collocation methods (12), using the results carried out in this paper. We first consider the case $m = 1$. According to Theorem 4.1, we choose $c_1 = \frac{5}{4}$, obtaining an order 2 A-stable method of the type (12) with

$$\chi(s) = \frac{5s - 2s^2}{4}, \tag{21}$$

$$\psi(s) = \frac{s(-1 + 2s)}{4}, \tag{22}$$

whose Butcher array (18) is

$$\left[\begin{array}{c|c}\mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V}\end{array}\right] = \left[\begin{array}{c|cc}\frac{25}{32} & 1 & \frac{15}{32} \\ \hline \frac{3}{4} & 1 & \frac{1}{4} \\ 1 & 0 & 0\end{array}\right]. \tag{23}$$

We next consider the case $m = 2$. According to Figure (1), we choose $c_1 = \frac{3}{2}$ and $c_2 = \frac{13}{5}$, obtaining an order 4 A-stable method of the type (12) with

$$\chi_1(s) = -\frac{s(-624 + 523s - 190s^2 + 25s^3)}{231}, \tag{24}$$

$$\chi_2(s) = \frac{-5s(-234 + 357s - 184s^2 + 30s^3)}{66}, \tag{25}$$

$$\psi_1(s) = \frac{s(-624 + 939s - 470s^2 + 75s^3)}{33}, \tag{26}$$

$$\psi_2(s) = \frac{5s(-48 + 79s - 48s^2 + 10s^3)}{462}, \tag{27}$$

whose Butcher array (18) is

$$\left[\begin{array}{c|c}\mathbf{A} & \mathbf{U} \\ \hline \mathbf{B} & \mathbf{V}\end{array}\right] = \left[\begin{array}{cc|ccc}\frac{1461}{1232} & \frac{225}{176} & 1 & -\frac{159}{176} & -\frac{75}{1232} \\ \frac{338}{275} & \frac{7267}{1650} & 1 & -\frac{2704}{825} & \frac{403}{1650} \\ \hline \frac{38}{33} & \frac{155}{66} & 1 & -\frac{80}{33} & -\frac{5}{66} \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0\end{array}\right]. \tag{28}$$

6. Numerical evidences

We now show some results arising from fixed stepsize numerical experiments, showing the effectiveness of the methods we have proposed.

We consider the following problem (see [14])

$$\begin{cases} y_1'(x) = -2y_1(x) + y_2(x) + 2\sin x \\ y_2'(x) = y_1(x) - 2y_2(x) + 2(\cos x - \sin x) \end{cases} \tag{29}$$

with $x \in [0, 10]$, with the initial condition $y(0) = [2, 3]^T$, whose exact solution is

$$\begin{cases} y_1(x) = 2e^{-x} + \sin x \\ y_2(x) = 2e^{-x} + \cos x. \end{cases} \tag{30}$$

We solve this problem using the two–step collocation method (28) with m=2 and uniform order 4. The results of the implementation are shown in table 1, where we have listed the number N of grid points we used, the global error $g(N)$ in the final point of the integration interval and the observed order of convergence p, computed from the formula

$$p = \frac{\log\left(ge(N)/ge(2N)\right)}{\log\left(2\right)}.$$

Table 1. Numerical results of the numerical solution of (29) with the method (28)

Method (28)		
N	ge	p
100	1.9705e-006	
200	1.0110e-007	4.2378
400	5.6576e-009	4.1594
800	3.3317e-010	4.0858
1600	1.9875e-011	4.0672

The table indicates the effectiveness of the derived methods and, moreover, confirms that the effective order of the method is 4. Further experiments, especially based on variable stepsize implementation of the derived methods, will be covered in papers in preparation.

7. Conclusions and future work

We have developed a new class of collocation based two-step Runge–Kutta methods (12) for the numerical solution of ordinary differential equations. These methods are of uniform order $p = 2m$ on the whole integration interval. We have discussed their stability properties, deriving A-stable methods with $m = 1, 2$ and order $p = 2, 4$ respectively. Examples of methods have also been provided and some preliminary numerical results have been shown.

Future work will address various implementation issues (e.g. the choice of appropriate starting procedures, stepsize and order changing strategy, solving nonlinear systems of equations by modified Newton methods and local error estimation) and also the extension of the collocation technique for methods of the type (2)-(3) using different basis of functions (e.g. trigonometrical, exponential or mixed basis), also in the context of second order ODEs (see [8,16,18,19]).

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