Collocation–based two step Runge–Kutta methods for Ordinary Differential Equations

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Abstract. We introduce a general family of collocation based two–step Runge–Kutta methods for the numerical integration of Ordinary Differential Equations depending on the stage values at two consecutive step points. We describe two constructive techniques and analyze the properties of the resulting methods.

1 Introduction

We are concerned with the numerical solution of an Initial Value Problem

$$\begin{cases} y'(x) = f(x, y(x)) \\ \\ y(x_0) = y_0 \end{cases} \tag{1}$$

through multistep collocation methods.

Let us assume that $x \in I := [x_0, X]$, and $f : I \times \Omega \subset \mathbb{R}^d \to \mathbb{R}^d$ is sufficiently smooth. Let $I_h = \{x_h : x_0 < x_1 < ... < x_N = X\}$ be a uniform grid on I, where $h = \frac{X - x_0}{N}$ is the stepsize. The new extension falls into the class of General Two Step Runge–Kutta methods (TSRK), introduced in [7], depending on the stage values at two consecutive step points, that is, in the autonomous case,

$$Y_n^j = u_j y_{n-1} + (1 - u_j) y_n + h \sum_{s=1}^{m} [a_{js} f(Y_{n-1}^s) + b_{js} f(Y_n^s)] \tag{2}$$

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

Here θ, v_j, w_j, a_{js}, b_{js}, $j,s,=1,\ldots,m$ are the coefficients of the methods, which can be represented by the following array:

$$\begin{array}{c|c|c} \mathbf{u} & \mathbf{A} & \mathbf{B} \\ \hline \theta & \mathbf{v^T} & \mathbf{w^T} \end{array} \tag{4}$$

These methods belong to the class of General Linear Methods, introduced by Butcher [1] with the aim to provide an unifying approach to analyze the classical subjects of consistency, convergence and stability of numerical methods for Ordinary Differential Equations (ODEs), which represents an active and increasing area of investigation [6].

The reason of interest in methods TSRK $(2,3)$ lies in the fact that, advancing from x_n to x_{n+1}, we only have to compute Y_n, because Y_{n-1} was already evaluated in the previous step. Therefore the computational cost of the method depends on the matrix B, while the matrix A adds extra degrees of freedom, without need for extra function evaluations. Therefore it is of interest to investigate the class of collocation based methods within the class of TSRK methods, in order to derive continuous methods with higher order of convergence, in comparison with classical collocation methods.

In Section 2 we recall the classical collocation methods, and also the extension to multistep methods already considered in the literature. In Section 3 we extend the idea of multistep collocations methods using two different constructive techniques, considering the two–step case. By adding some extra collocation conditions, the resulting methods depend on the stage values at two consecutive step points and provide a uniform approximation to the solution of order $2m+1$, where m is the number of stages. In Section 4 we analyze the linear stability properties of the methods. In Section 5 we describe some numerical experiments.

2 Classical one step and multistep collocation methods

The idea of collocation is old and well known in Numerical Analysis [9, 4, 5]. In order to advance from x_n to x_{n+1}, an algebraic polynomial $P(x)$ is constructed, which interpolates the numerical solution in the step point x_n, and satisfies the ODEs in the points x_n+c_ih, where $\{c_1,c_2,...,c_m\}$ are m real numbers (typically between 0 and 1), that is

$$\begin{cases} P(x_n)=y_n, \\ P'(x_n+c_ih)=f(x_n+c_ih,P(x_n+c_ih)), \quad i=1,2,...,m. \end{cases} \tag{5}$$

The solution in x_{n+1} is given by

$$y_{n+1}=P(x_{n+1}). \tag{6}$$

It is known that one step collocation methods are a subset of implicit Runge-Kutta methods

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & & a_{1m} \\ c_2 & a_{21} & a_{22} & & a_{2m} \\ \\ ... & ... & ... & & ... \\ \\ c_m & a_{m1} & a_{m2} & & a_{mm} \\ \hline & b_1 & b_2 & & b_m \end{array}$$

where

$$a_{ij} = \int_0^{c_i} L_j(t)dt, \qquad b_j = \int_0^1 L_j(t)dt, \qquad i,j = 1,2,...,m \tag{7}$$

and $L_j(t)$, $j = 1,...,m$, are fundamental Lagrange polynomials. Moreover the maximum attainable order is at most $2m$, and it i s obtained by using Gaussian collocation points [9, 4]. Guillou and Soulé introduced multistep collocation methods [3], by adding interpolation conditions in the previous k step points, so that the collocation polynomial is defined by

$$\begin{cases} P(x_{n-i}) = y_{n-i} \quad i = 0,1,...,k-1, \\ \\ P'(x_n + c_j h) = f(x_n + c_j h, P(x_n + c_j h)) \quad j = 1,...,m. \end{cases} \tag{8}$$

The numerical solution is then

$$y_{n+1} = P(x_{n+1}) \tag{9}$$

In [5] it is proved that this method is equivalent to a multistep Runge–Kutta method, and the points which guarantee superconvergence are called Radau points. Lie and Norsett analyze the order of the resulting methods [10].

3 General two–step collocation methods

We now extend the idea of multistep collocation methods, by considering the case of $k = 2$, and by adding some extra collocation conditions, so that the resulting methods depend on the stage values at two consecutive step points. We extend the technique used by Hairer and Wanner [5]. In more detail, the collocation polynomial is then defined by the following conditions:

$$\begin{cases} P(x_{n-1}) = y_{n-1}, \\ \\ P(x_n) = y_n, \\ \\ P'(x_{n-1} + c_i h) = f(x_{n-1} + c_i h, P(x_{n-1} + c_i h)), \quad i = 1,2,...,m, \\ \\ P'(x_n + c_i h) = f(x_n + c_i h, P(x_n + c_i h)), \quad i = 1,2,...,m. \end{cases} \tag{10}$$

The previous problem constitutes a Hermite interpolation problem with incomplete data (because the function values $P(x_{n-1}+c_jh)$, $P(x_n+c_jh)$ are missing). In order to compute the collocation polynomial we introduce the generalized Lagrange basis

$$\{\overline{\phi}_i(x), \overline{\chi}_j(x), \overline{\psi}_j(x), \quad i=0,1, \quad j=1,2,...,m\}$$

such that the collocation polynomial is expressed in the following way:

$$\begin{aligned} P(x) = {} & \overline{\phi}_0(x)y_{n-1} + \overline{\phi}_1(x)y_n + \\ & + h\sum_{j=1}^{m}\left[\overline{\chi}_j(x)P'(x_{n-1}+c_jh) + \overline{\psi}_j(x)P'(x_n+c_jh)\right], \end{aligned} \tag{11}$$

Introducing the dimensionless coordinate $t = \frac{x-x_n}{h}$, the collocation polynomial takes the form

$$\begin{aligned} P(x_n+th) = {} & \phi_0(t)y_{n-1} + \phi_1(t)y_n + \\ & + h\sum_{j=1}^{m}\left[\chi_j(t)P'(x_{n-1}+c_jh) + \psi_j(t)P'(x_n+c_jh)\right]. \end{aligned} \tag{12}$$

We must exhibit the expression of the basis functions $\phi_i(t)$ $(i=0,1)$, $\psi_j(t)$ and $\chi_j(t)$ $(j=1,2,...m)$. They can be obtained by applying the interpolation conditions

$$\begin{aligned} & \phi_0(t_0)=1,\, \phi_0(t_1)=0,\, \phi_1(t_0)=0,\, \phi_1(t_1)=1, \\ & \chi_i(t_l)=0,\; \psi_i(t_l)=0, \end{aligned} \tag{13}$$

and the collocation ones

$$\begin{aligned} & \phi_0'(c_i-1)=0, \quad \phi_0'(c_i)=0,\, \phi_1'(c_i-1)=0,\, \phi_1'(c_i)=0, \\ & \chi_j'(c_i-1)=\delta_{ij},\, \chi_j'(c_i)=0,\, \psi_j'(c_i-1)=0,\, \psi_j'(c_i)=\delta_{ij}, \end{aligned} \tag{14}$$

where $t_0=-1$, $t_1=0$, $l=0,1$, $i,j=1,2,\ldots,m$.

Theorem 1. *The method defined by (10) is equivalent to a two–step Runge–Kutta method [7]*

$$\begin{aligned} Y_n^j &= u_jy_{n-1} + (1-u_j)y_n + h\sum_{s=1}^{m}[a_{js}f(x_{n-1}+c_sh, Y_{n-1}^s) \\ &\quad + b_{js}f(x_n+c_sh, Y_n^s)], \quad j=1,...,m, \\ y_{n+1} &= \theta y_{n-1} + (1-\theta)y_n + h\sum_{j=1}^{m}[v_jf(x_{n-1}+c_jh, Y_{n-1}^j) \\ &\quad + w_jf(x_n+c_jh, Y_n^j)]. \end{aligned}$$

where

$$\begin{aligned} & \theta=\phi_0(1), \quad v_j=\chi_j(1), \;\; w_j=\psi_j(1), \\ & b_{js}=\psi_j(c_s),\, u_j=\phi_0(c_j),\, a_{js}=\chi_j(c_s),\, j,s=1,...,m. \end{aligned}$$

Proof. In order to compute the polynomials $\phi_i(t)$, $\chi_j(t)$, $\psi_j(t)$, we follow the procedure indicated in [5]. We first expand the basis polynomials in the following form

$$\phi_i(t) = \sum_{l=0}^{2m+1} d_l^{(i)} t^l, \qquad i = 1, 2 \tag{15}$$

$$\chi_j(t) = \sum_{l=0}^{2m+1} p_l^{(j)} t^l, \qquad \psi_j(t) = \sum_{l=0}^{2m+1} q_l^{(j)} t^l \qquad j = 1, ..., m \tag{16}$$

Applying (13), (14) in (15), (16) we obtain the following $2m + 2$ linear systems:

$$Hd^{(i)} = N_1, \quad i = 1, 2, \tag{17}$$

$$Hp^{(i)} = N_2, \quad Hq^{(i)} = N_3 \quad i = 1, ..., m, \tag{18}$$

where H is the coefficient matrix

$$H = \begin{pmatrix} 1 & t_0 & t_0^2 & ... & ... & t_0^{2m+1} \\ 1 & t_1 & t_1^2 & ... & ... & t_1^{2m+1} \\ 0 & 1 & 2(c_1-1) & 3(c_1-1)^2 & ... & (2m+1)(c_1-1)^{2m} \\ ... & ... & & & & \\ ... & ... & & & & \\ 0 & 1 & 2(c_m-1) & 3(c_m-1)^2 & ... & (2m+1)(c_m-1)^{2m} \\ 0 & 1 & 2c_1 & 3c_1^2 & ... & (2m+1)c_1^{2m} \\ ... & ... & & & & \\ ... & ... & & & & \\ 0 & 1 & 2c_m & 3c_m^2 & ... & (2m+1)c_m^{2m} \end{pmatrix}.$$

N_1, N_2, N_3 are the following vectors

$$N_1 = [\delta_{i1}, \delta_{i2}, 0, ..., 0]^T, \quad N_2 = [0, 0, \delta_{i1}, ..., \delta_{im}, 0, ..., 0]^T$$
$$N_3 = [0, ..., 0, \delta_{i1}, ..., \delta_{im}]^T$$

and $d^{(i)}, p^{(i)}$, $q^{(i)}$ are the unknowns vectors. These linear systems can be solved (apart from some exceptional values of the collocation abscissa), giving the expressions of the collocation polynomial $P(x)$. □

Each linear system arising in the construction of these methods is nonsingular, because its coefficient matrix is of Vandermonde type. We omit the details of the proof, simply because it uses the well-known technique applied in computing the determinant of the Vandermonde matrix [11].

3.1 Another constructive technique

Let us extend the technique used by Lie and Norsett [10] in order to derive general two–step Runge–Kutta methods of collocation type.

Theorem 2. *The method defined by (10) is equivalent to a two–step Runge–Kutta method having the following form:*

$$Y_n^j = \phi_0(c_s)y_{n-1} + \phi_1(c_s)y_n + h\sum_{s=1}^{m}[\chi_j(c_s)f(x_{n-1}+c_sh, Y_{n-1}^s) + \psi_j(c_s)f(x_n+c_sh, Y_n^s)], \quad j=1,\dots,m, \tag{19}$$

$$y_{n+1} = \phi_0(1)y_{n-1} + \phi_1(1)y_n + h\sum_{j=1}^{m}[\chi_j(1)f(x_{n-1}+c_jh, Y_{n-1}^j) + \psi_j(1)f(x_n+c_jh, Y_n^j)], \tag{20}$$

where

$$\psi_j(t) = \int_0^t l_j(\tau)d\tau - \frac{\int_{-1}^0 l_j(\tau)d\tau}{\int_{-1}^0 M(\tau)d\tau}\int_0^t M(\tau)d\tau, \quad j=1,\dots,m, \tag{21}$$

$$\chi_j(t) = \int_0^t \tilde{l}_j(\tau)d\tau - \frac{\int_{-1}^0 \tilde{l}_j(\tau)d\tau}{\int_{-1}^0 M(\tau)d\tau}\int_0^t M(\tau)d\tau, \quad j=1,\dots,m, \tag{22}$$

$$\phi_0(t) = -\frac{\int_0^t M(\tau)d\tau}{\int_{-1}^0 M(\tau)d\tau}, \tag{23}$$

$$\phi_1(t) = 1 + \frac{\int_0^t M(\tau)d\tau}{\int_{-1}^0 M(\tau)d\tau}. \tag{24}$$

with

$$l_i(t) = \prod_{j=1, j\neq i}^{2m}\frac{t-d_j}{d_i-d_j}, \qquad M(t) = \prod_{j=1}^{2m}(t-d_j), \qquad \begin{cases} d_i = c_i \\ d_{m+i} = c_i - 1, \end{cases} \quad i=1,2,...,m \tag{25}$$

$$\tilde{l}_j(t) = \prod_{i=1, i\neq j}^{2m}\frac{t-e_i}{e_j-e_i}, \qquad \begin{cases} e_i = c_i - 1 \\ e_{m+i} = c_i, \end{cases} \qquad = 1,2,...,m$$

Proof. To prove that the general two–step collocation method defined by (10) is equivalent to the TSRK method (19)-(20), we must exhibit the form of the basis polynomials $\phi_i(x)$ $(i=0,1)$, $\psi_j(x)$ and $\chi_j(x)$ $(j=1,2,...m)$. We use the scaled time variable t.

- We first consider $\psi_j(t)$, $j = 1, 2, ...m$.

The interpolation and collocation conditions on ψ_j are

$$\begin{aligned} \psi_j(-r) &= 0, \qquad r = 0, 1 \\ \psi_j'(c_s - 1) &= 0, \qquad s = 1, ..., m \\ \psi_j'(c_s) &= \delta_{js}, \qquad s = 1, ..., m. \end{aligned}$$

We denote the collocation knots in the following way:

$$\begin{cases} d_i = c_i \\ d_{m+i} = c_i - 1, \qquad i = 1, 2, ..., m. \end{cases}$$

Therefore the previous conditions on ψ_j are

$$\psi_j(-r) = 0, \qquad r = 0, 1, \tag{26}$$

$$\psi_j'(d_s) = \Delta_{js}, \qquad s = 1, ..., 2m. \tag{27}$$

where

$$\Delta_{js} = \begin{cases} \delta_{js}, & \text{if } 1 \le s \le m \\ 0, & \text{else.} \end{cases} \tag{28}$$

Following [10], the collocation conditions can be satisfied by a polynomial of the form

$$\psi_j'(t) = l_j(t) + \frac{\alpha_0}{a_j} M(t) \tag{29}$$

with

$$l_j(t) = \prod_{i=1, i \neq j}^{2m} \frac{t - d_i}{d_j - d_i}, \qquad M(t) = \prod_{j=1}^{2m} (t - d_j)$$

$$a_j = \prod_{s=1, s \neq j}^{2m} (d_j - d_s), \qquad \alpha_0 \in \mathbb{R}.$$

Setting $\bar{\alpha}_0 = \frac{\alpha_0}{a_j}$, equation (29) becomes

$$\psi_j'(t) = l_j(t) + \bar{\alpha}_0 M(t). \tag{30}$$

Integrating the last equation, we find

$$\psi_j(t) = \int_0^t l_j(\tau) d\tau + \bar{\alpha}_0 \int_0^t M(\tau) d\tau. \tag{31}$$

Imposing the interpolation conditions (26), we compute $\bar{\alpha}_0$ by solving the linear equation

$$\bar{\alpha}_0 \int_{-1}^0 M(\tau) d\tau = - \int_{-1}^0 l_j(\tau) d\tau. \tag{32}$$

For $\psi_j(t)$ we have

$$\psi_j(t) = \int_0^t l_j(\tau)d\tau - \frac{\int_{-1}^0 l_j(\tau)d\tau}{\int_{-1}^0 M(\tau)d\tau} \int_0^t M(\tau)d\tau. \tag{33}$$

• We then consider $\chi_j(t)$, $j = 1, 2, ...m$.
The proof is the same as above, putting

$$\begin{cases} e_i = c_i - 1 \\ e_{m+i} = c_i, \qquad = 1, 2, ..., m \end{cases}$$

instead of d_i, $i = 1, ..., 2m$.
• We now consider $\phi_i(t)$ $(i = 0, 1)$.
Using collocation knots d_j, for ϕ_i we have:

$$\phi_i(-r) = 1 - \delta_{ir} \qquad r = 0, 1, \tag{34}$$

$$\phi_i'(d_j) = 0 \qquad j = 1, ..., m. \tag{35}$$

The previous conditions are then verified by

$$\phi_i(t) = \gamma_0^{(i)} + \gamma_1^{(i)} \int_0^t M(\tau)d\tau,$$

where $M(t) = \prod_{j=1}^{2m}(t - d_j)$ and $\gamma_j^{(i)} \in \mathbb{R}$. First of all we consider ϕ_0:

$$\phi_0(t) = \gamma_0^{(0)} + \gamma_1^{(0)} \int_0^t M(\tau)d\tau.$$

We know that

$$0 = \phi_0(0) = \gamma_0^{(0)} + \gamma_1^{(0)} \int_0^0 M(\tau)d\tau$$

so we have $\gamma_0^{(0)} = 0$. Moreover, it is

$$1 = \phi_0(-1) = \gamma_1^{(0)} \int_0^{-1} M(\tau)d\tau = -\gamma_1^{(0)} \int_{-1}^0 M(\tau)d\tau \tag{36}$$

therefore we obtain

$$\gamma_1^{(0)} = -\frac{1}{\int_{-1}^0 M(\tau)d\tau}. \tag{37}$$

To conclude the proof we must exhibit the basis polynomial $\phi_1(t)$. As for $\phi_0(t)$, we impose the interpolation conditions (34), obtaining

$$1 = \phi_1(0) = \gamma_0^{(1)}$$

while, applying the collocation ones (35), it is

$$0 = \phi_1(-1) = \gamma_0^{(1)} + \gamma_1^{(1)} \int_0^{-1} M(\tau)d\tau = 1 - \gamma_1^{(1)} \int_{-1}^0 M(\tau)d\tau. \tag{38}$$

So, we arrive to the following expression of the coefficients of $\phi_1(t)$:

$$\gamma_0^{(1)} = 1, \qquad \gamma_1^{(1)} = \frac{1}{\int_{-1}^{0} M(\tau)d\tau}. \tag{39}$$

□

3.2 Order results

It is now possible to prove that $P(x)$ provides a uniform approximation to the solution of order $2m+1$ for any choice of the collocation abscissa $\{c_1, c_2, ..., c_m\}$. In particular, the following theorem deals with the order conditions.

Theorem 3. *Let*

$$G_i = det \begin{pmatrix} \int_{-1}^{0} M(\tau)\tau^i d\tau & \int_{-1}^{0} M(\tau)\tau^{i+1} d\tau \\ \int_{0}^{1} M(\tau)\tau^i d\tau & \int_{0}^{1} M(\tau)\tau^{i+1} d\tau \end{pmatrix}. \tag{40}$$

Then the general m stages collocation method has order $2m+\sigma$ if and only if $G_i = 0$ for $i = 0, 1, \ldots, \sigma - 1$.

Proof. The proof uses Alekseev–Gröbner theorem and the knots d_i defined by (25). Technical details are given in [10]. □

The following theorem concerns the possibility to achieve superconvergence.

Theorem 4. *The maximum attainable order of a two–steps and m stages collocation method arising from (10) is $3m$.*

Proof. The set of conditions $G_i = 0$ of theorem 3 gives a nonlinear system in the unknowns $c_1, c_2, ..., c_m$. Let us consider a subset $\Gamma(\zeta)$ of s equations of the system, where $\Gamma(\zeta) : \mathbb{R}^m \to \mathbb{R}^s$, which has unique solution if and only if $s = m$. As a consequence, σ can be at most equal to m and, for this reason, the maximum attainable order is $3m$. □

4 Linear Stability Analysis

From [6], we recall that a TSRK method (2)-(3)

$$Y_i^{[n]} = (1-u_i)y_n + u_i y_{n-1} + h\sum_{j=1}^{m}(a_{ij}f(Y_j^{[n]}) + b_{ij}f(Y_j^{[n-1]}))$$

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

is a General Linear Method of the form

$$\left[\begin{array}{c} Y^{[n]} \\ \hline y_{n+1} \\ y_n \\ hf(Y^{[n]}) \end{array}\right] = \left[\begin{array}{c|ccc} A & e-u & u & B \\ \hline v^T & 1-\theta & \theta & w^T \\ 0 & 1 & 0 & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{array}\right] \left[\begin{array}{c} hf(Y^{[n]}) \\ \hline y_n \\ y_{n-1} \\ hf(Y^{[n-1]}) \end{array}\right], \tag{41}$$

where $\mathbf{I}$ is the identity matrix whose dimension is the number of stages and $\mathbf{0}$ is the zero matrix or vector of appropriate dimensions. The stability (or amplification) matrix $M(z)$ associated to this method takes the form (compare with [6])

$$M(z) = \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 1 & 0 & \mathbf{0} \\ zS(z)(\mathbf{e}-u) & zS(z)u & zS(z)B \end{bmatrix} \tag{42}$$

where

$$\begin{aligned} M_{11} &= 1-\theta+zv^TS(z)(\mathbf{e}-u), \\ M_{12} &= \theta+zv^TS(z)u, \\ M_{13} &= w^T+zv^TS(z)B, \end{aligned}$$

$S(z) = (I-zA)^{-1}$, $\mathbf{e}$ is the vector with unitary entries. Let us consider our class of methods for $m=1$. The matrix representing these methods has the form

$$\left[\begin{array}{c|ccc} a & 1-u & u & b \\ \hline v & 1-\theta & \theta & w \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{array}\right] = \left[\begin{array}{c|ccc} \chi(c) & 1-\phi_0(c) & \phi_0(c) & \psi(c) \\ \hline \chi(1) & 1-\phi_0(1) & \phi_0(1) & \psi(1) \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{array}\right] \tag{43}$$

and the amplification matrix has the form

$$M(z) = \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ 1 & 0 & 0 \\ zS(z)(1-\phi_0(c)) & zS(z)\phi_0(c) & zS(z)\psi(c) \end{bmatrix} \tag{44}$$

where

$$\begin{aligned} M_{11} &= 1-\phi_0(1)+z\chi(1)S(z)(1-\phi_0(c)), \\ M_{12} &= \phi_0(1)+z\chi(1)S(z)\phi_0(c), \\ M_{13} &= \psi(1)+z\chi(1)S(z)\psi(c). \end{aligned}$$

We perform a numerical search to find collocation abscissae to get wide stability regions. For $c=1$, using the boundary locus technique, we obtain the stability region plotted in fig. 1.

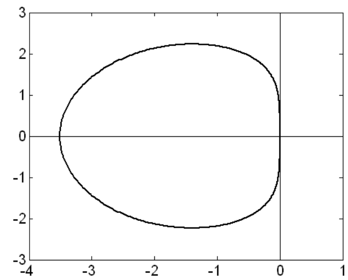

Fig. 1. Stability region of one-stage method for $c = 1$.

In particular, the stability interval of this method is $[-\frac{79}{20}, 0]$.

Let us look at two–stage methods. These methods are represented by the following array

$$\left[\begin{array}{cc|cccc} a_{11} & a_{12} & 1-u_1 & u_1 & b_{11} & b_{12} \\ a_{21} & a_{22} & 1-u_2 & u_2 & b_{21} & b_{22} \\ v_1 & v_2 & 1-\theta & \theta & w_1 & w_2 \\ \hline 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{array}\right] \qquad (45)$$

Fig. 2 shows the stability region of the two–stage method associated to $c_1 = \frac{1}{2}$ and $c_2 = 1$. In this case, the stability interval is $[-\frac{14}{5}, 0]$.

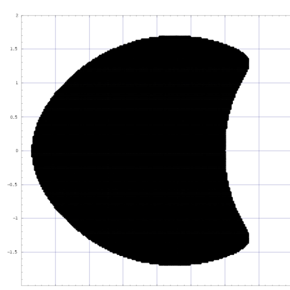

Fig. 2. Stability region of two-stage method for $c_1 = \frac{1}{2}$ and $c_2 = 1$.

5 Numerical experiments

We have tested our class of methods on many non-stiff and stiff problems. We

present below a selection of results of numerical experiments with fixed stepsize, designed to compare our methods with respect to classical one step collocation Runge–Kutta methods. Even if our methods have no unbounded stability regions, they can be suitable to integrate also stiff problems, just by adapting the choice of the step size to the amplitude of the interval of stability. Indeed, methods having unbounded stability regions, for example A-stable methods, can integrate stiff problems also with larger step size, but this kind of integration could highten the error committed too much.
The numerical experiments are carried over with a fixed stepsize, without the usage of strategies to save function evaluations.

We first consider the following linear problem (cfr. [9])

$$\begin{cases} y_1'(x) = -2y_1(x) + y_2(x) + 2\sin x \\ y_2'(x) = y_1(x) - 2y_2(x) + 2(\cos x - \sin x) \end{cases} \tag{46}$$

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

$$\begin{cases} y_1(x) = 2e^{-x} + \sin x \\ y_2(x) = 2e^{-x} + \cos x \end{cases}. \tag{47}$$

We solve this problem using the general two–step collocation method defined in theorem 1 and in (19)-(20) with $m = 1$ and $c = 1$ (GTSCOLL) and we compare it with the one step Gauss method with one stage (of order 2) and the Radau IIA with 2 stages (of order 3), in order to have a comparison between methods having the same number of stages (Gauss) and the same order (Radau IIA) and also with BDF method of order 3 (BDF), which is usually considered a standard method for stiff problems [8]. The result of the implementation is shown in the following tables, where h is the step size used, fe is the number of function evaluations, cd is the number of correct digits, ge is the global error committed at the end of the integration interval.

GTSCOLL method, m=1, p=3			
h	fe	cd	ge
0.1	2242	4.9435	1.1387e-005
0.05	3522	5.8438	1.4328e-006
0.025	5866	6.7454	1.7968e-007
0.0125	9580	7.6491	2.2430e-008
0.00625	18144	8.5507	2.8133e-009
0.003125	31984	9.4569	3.4917e-010

Gauss method, m=1, p=2			
h	fe	cd	ge
0.1	297	3.0565	8.7792e-004
0.05	597	3.6588	2.1936e-004
0.025	1197	4.2609	5.4835e-005
0.0125	2397	4.8630	1.3708e-005
0.00625	4797	5.4650	3.4270e-006
0.003125	9597	6.0671	8.5676e-007

Radau IIA method, m=2, p=3			
h	fe	cd	ge
0.1	2966	4.7535	1.7637e-005
0.05	4750	5.6481	2.2484e-006
0.025	7904	6.5468	2.8386e-007
0.0125	12972	7.4478	3.5660e-008
0.00625	25036	8.3497	4.4689e-009
0.003125	44684	9.2523	5.5928e-010

BDF method, k=3, p=3			
h	fe	cd	ge
0.1	198	4.0413	9.0920e-005
0.05	398	4.9149	1.2163e-005
0.025	798	5.8036	1.5716e-006
0.0125	1598	6.6996	1.9968e-007
0.00625	3190	7.5992	2.5163e-008
0.003125	3708	8.5006	3.1579e-009

As shown in fig. 3, the method GTSCOLL gives the best accuracy. If we compare the results obtained by our method and the Gauss one, we can see that the GTSCOLL method, using the same number of stages, gives a higher order of accuracy. If compared with the Radau IIA method with same order, but with two stages, our method gives a better accuracy as well. BDF method gives less accurate results, by using less function evaluations.

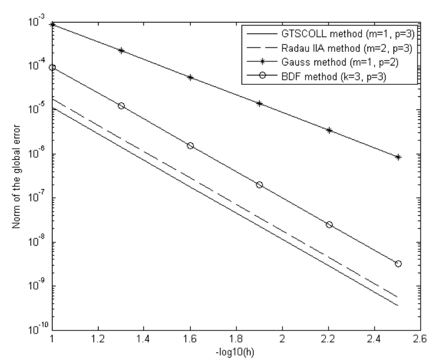

Fig. 3. Comparison between three solvers for the problem (46).

We next consider the well known Van der Pol's equation [5]. We reduce this second order ODE to the following first order system of two equations

$$\begin{cases} y_1' = y_2 \\ y_2' = \mu(1 - y_1^2)y_2 - y_1 \end{cases} \tag{48}$$

with $x \in [0, 100]$ and with the initial condition $y(0) = [2, 0]^T$. In particular, we consider the case $\mu = 1000$. The parameter $\mu > 0$ hightens the importance of the nonlinear part of the equation. This problem exhibits a particular phenomenon: the problem switches from stiff to nonstiff with a very sharp changing solution. This makes the equation quite challenging for ODEs solvers.

The GTSCOLL method, having a bounded stability region, is able to integrate this nonlinear stiff problem using a stepsize adapted to the amplitude of the stability region: in particular, it shows the same behaviour of the Gauss method and it is better than the Radau and BDF methods:

GTSCOLL method			
h	fe	cd	ge
0.1	1889	6.8483	1.4180e-007
0.05	3098	6.8870	1.2971e-007

Gauss method			
h	fe	cd	ge
0.1	2996	6.9023	1.2520e-007
0.05	5996	6.9023	1.2520e-007

Radau IIa method			
h	fe	cd	ge
0.1	13010	4.1495	7.0869e-005
0.05	24010	4.4498	3.5496e-005

BDF method			
h	fe	cd	ge
0.1	1554	6.9013	1.2509e-007
0.05	3108	6.9029	1.2510e-007

In many cases, it is possible to give an upper bound for the stepsize, in order to integrate a stiff system also with methods having a bounded stability interval. We show an example in which we obtain such an estimation of the stepsize. The following problem is Kramarz's system [8], which is often used in numerical experiments on periodic stiffness (cfr. [14]) on second order ODEs:

$$y''(x) = Ay(x) = \begin{pmatrix} 2498 & 4998 \\ -2499 & -4999 \end{pmatrix} y(x), \tag{49}$$

where A is the matrix of coefficients in (49), $y(x) = [y_1(x), y_2(x)]^T$, with $y(0) = [2, -1]^T$ and $x \in [0, 2\pi]$. The exact solution of this problem is

$$y(x) = \begin{pmatrix} 2\cos x \\ -\cos x \end{pmatrix}. \tag{50}$$

The eigenvalues of A are $\lambda_1 = -2500$, $\lambda_2 = -1$; then the analytical solution of the system exhibits the two frequencies 1 and $\sqrt{2500}$, but the high frequency component is eliminated by the initial conditions. Notwithstanding this, its presence in the general solution of the system dictates restrictions on the choice of the stepsize, so that the system is stiff.

We transform this problem in a system of 4 ordinary differential equations of the first order and we integrate it by using the GTSCOLL method, whose stability interval is $[-\frac{79}{20}, 0]$. In order to get stable results, the product $h\lambda$ must be in $[-\frac{79}{20}, 0]$, so $h \leq \frac{79}{50000} = 0.00158$. If we use a stepsize $h \leq 0.00158$, the GTSCOLL method integrates the above problem with a bounded error. The following table shows that this actually happens. Then we compare these results with the one obtained by the Gauss method.

GTSCOLL method			
h	fe	cd	ge
0.00158	19883	2.6095	2.4575e-3
0.00079	39768	3.1539	7.0154e-4
0.000395	79533	3.1523	7.0418e-4
0.0001975	159068	3.5797	2.6320e-4
0.00009875	318138	4.3710	4.2559e-5
0.000049375	636273	4.3706	4.2600e-5

Gauss method			
h	fe	cd	ge
0.00158	19873	2.6065	2.4745e-3
0.00079	39726	3.1513	7.0579e-4
0.000395	79237	3.1517	7.0523e-4
0.0001975	156735	3.5793	2.6347e-4
0.00009875	298833	4.3703	4.2624e-5
0.000049375	509014	4.3704	4.2616e-5

BDF method			
h	fe	cd	ge
0.00158	6543	2.6070	2.4715e-3
0.00079	9694	3.1517	7.0504e-4
0.000395	15906	3.1517	7.0504e-4
0.0001975	31813	3.5793	2.6342e-4
0.00009875	63627	4.3704	4.2613e-5
0.000049375	127254	4.3706	4.2607e-5

Actually our collocation method shows the same behaviour of the Gauss method and BDF method, despite of its bounded stability region.

6 Conclusions

We presented the family of collocation–based General Two Step Runge–Kutta methods for $y' = f(x, y)$, which exhibit high order of convergence, and high stage order. The knowledge of the collocation polynomial, which provides a uniform approximation in any point of the integration interval, may allow their usage in a variable stepsize implementation, so that they seem promising for future development.

In order to overcome the limit of a limited stability regions, a modification of the collocation approach by relaxing some collocation conditions is under development in [2], to derive A–stable methods of lower order within the same family.

It is also the purpose of our research to investigate on the use of different classes of function basis (cfr. [12]), e.g. trigonometric polynomials, exponentials or mixed basis, in order to obtain continuous methods which are particularly suitable to integrate problems having periodic or oscillatory solutions.

Acknowledgments

We wish to thank Prof. Zdzislaw Jackiewicz for his helpful and valuable discussions and comments along time on various issues in the field.

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