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Research Article

High order second derivative multistep collocation methods for ordinary differential equations

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Abstract

In this paper, we introduce second derivative multistep collocation methods for the numerical integration of ordinary differential equations (ODEs). These methods combine the concepts of both multistep methods and collocation methods, using second derivative of the solution in the collocation points, to achieve an accurate and efficient solution with strong stability properties, that is, A-stability for ODEs. Using the second-order derivatives leads to high order of convergency in the proposed methods. These methods approximate the ODE solution by using the numerical solution in some points in the r previous steps and by matching the function values and its derivatives at a set of collocation methods. Also, these methods utilize information from the second derivative of the solution in the collocation methods. We present the construction of the technique and discuss the analysis of the order of accuracy and linear stability properties. Finally,

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some numerical results are provided to confirm the theoretical expectations. A stiff system of ODEs, the Robertson chemical kinetics problem, and the two-body Pleiades problem are the case studies for comparing the efficiency of the proposed methods with existing methods.

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1 Introduction

This paper is devoted to introducing a new class of collocation methods by using the second derivative of the solution for the numerical solution of ordinary differential equations (ODEs) in the form

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

where the function $f : \mathbb{R}^d \longrightarrow \mathbb{R}^d$ is sufficiently smooth, $y_0 \in \mathbb{R}^d$ is a known initial value, and the dimensionality of the system is shown by d.

One-step collocation methods for ODEs have been analyzed by many authors (see [3] and references therein contained). As it is well known, the collocation methods is a technique that the given equation is transformed to an algebraic equation by representing the solution as a combination of basic functions belonging to a chosen finite dimensional space, usually a piecewise algebraic polynomial, which enforces the integral equation at the chosen collocation points.

Multistep methods play a crucial role in the numerical integration of ODEs due to their ability to obtain the approximate solution of a high order of convergence. Lie and Nørsett [14] first introduced the idea of multistep collocation methods. In comparison with classical collocation methods, these methods depend on more parameters while computational cost does not exceed them, and these methods have high convergence order and strong stability properties.

In comparison with one-step methods, in view of computational cost and precision of approximation, the multistep methods are more efficient [13].

Using higher order derivative can be a helpful way to achieve the integration methods will be more stable with high order convergency in both onestep and multistep methods. Firstly, a class of second-order derivative formulas is created, and the stability of these formulas was investigated by Enright [7]. Following this work, successful implementation of second-order derivatives has been developed in many literatures [4, 5, 6]. Also, second derivative two-step collocation methods have been recently constructed in [8]. These methods and all other traditional second derivative methods can be considered as special cases of the class of second derivative general linear methods (see, for instance, [1, 2, 4]).

We aim to provide a second derivative extension of the multistep collocation methods (SDMCMs) that use the second derivatives of the solution in the collocation points. These methods combine the advantages of both multistep collocation methods and second derivative methods to obtain methods with higher order accuracy and desired stability properties. In other word, we derive a special case of multistep collocation methods, which fixed number r of previous time steps and first and second derivative of the solution in m collocation points are used in the approximation of the solution in every subinterval. The advantages of these methods are their ability to handle stiff ODEs and their superior accuracy compared to multistep collocation methods while the computational cost does not exceed.

Theoretical concepts of new proposed methods, SDMCMs, is discussed in details in Section 2. In Section 3, the order condition of the proposed method is obtained. Section 4 is dedicated to analyzing the linear stability properties of SDMCMs with respect to the linear basic test equation. The proposed methods with two and three steps and one and two collocation parameters are constructed in Section 5. Finally, Section 6 presents several numerical examples in order to validate the effectiveness of proposed methods and experimentally verify the order of convergence.

2 Construction of method

Let us divide the interval $I := [t_0, T]$ to the finite set of subintervals $[t_n, t_{n+1}]$ for $n = 0, 1, \ldots, N-1$ by introducing a uniform mesh h in the form

$$I_h = \{t_0 + nh|\ n = 0, 1, \ldots, N,\ h > 0, \quad Nh = T - t_0\}.$$

Also, consider the abscissa vector $c = [c_1, c_2, \ldots, c_m]^T$ and define the collocation parameters by $t_{n,i} := t_n + c_i h$. The multi-step continuous approximation to the solution of (1) is defined by

$$\begin{cases} P(t_n + sh) = \displaystyle\sum_{k=0}^{r-1} \varphi_k(s) y_{n-k} + h \sum_{j=1}^{m} \Big(\psi_j(s) f(P(t_{n,j}))\Big) \\ \qquad\qquad + h^2 \displaystyle\sum_{j=1}^{m} \Big(\chi_j(s) g(P(t_{n,j}))\Big), \\ y_{n+1} = P(t_{n+1}), \end{cases} \tag{2}$$

with $s \in (0, 1]$ and the function g is the second derivative of unknown function $y(t)$ and is defined by $g(\cdot) = f'(\cdot)f(\cdot)$. Also, for the implementation of the method, the approximate solution in the initial interval $[t_0, t_{r-1}]$ is needed where can be computed by an arbitrary method with sufficiently high order convergency . The method is defined by the coefficient functions $\varphi_k(s),\ \psi_j(s),\ \chi_j(s)$, $j = 1, \ldots, m$, $k = 0, 1, \ldots, r-1$, which are polynomials of degree $2m + r - 1$. The interpolation conditions for $P(t_n + sh)$ at the points t_{n-i}, lead to

$$P(t_{n-i}) = y_{n-i}, \quad i = 0, 1, \ldots, r-1, \tag{3}$$

and collocating the both sides of (1) and its derivative in the collocation points $t_{n,i}$ is written in the form

$$P'(t_{n,i}) = f(P(t_{n,i})), \quad P''(t_{n,i}) = g(P(t_{n,i})), \quad i = 1, 2, \ldots, m. \tag{4}$$

The coefficient polynomials of method are determined by conditions (3) and (4), which lead to

$$\varphi_k(-i) = \delta_{ik},\ \ \psi_j(-i) = 0, \quad \chi_j(-i) = 0, \tag{5}$$

and

$$\begin{aligned} &\varphi_k'(c_i) = 0, \quad \psi_j'(c_i) = \delta_{ij}, \quad \chi_j'(c_i) = 0, \\ &\varphi_k''(c_i) = 0, \quad \psi_j''(c_i) = 0, \quad \chi_j''(c_i) = \delta_{ij}, \end{aligned} \tag{6}$$

where δ_{ij}, $i, j = 1, 2, \ldots, m$, is the usual Kronecker delta. The construction of these polynomials is obtained by the Hermite–Birkhoff interpolation [18]. To find the unique polynomial that satisfies these conditions, the polynomials $\varphi_k(s)$, $\psi_j(s)$, and $\chi_j(s)$ can be formulated in the form

$$\varphi_k(s) = \sum_{i=0}^{2m+r-1} \Phi_i^{[k]} \frac{s^i}{i!}, \quad \psi_j(s) = \sum_{i=0}^{2m+r-1} \Psi_i^{[j]} \frac{s^i}{i!}, \quad \chi_j(s) = \sum_{i=0}^{2m+r-1} \chi_i^{[j]} \frac{s^i}{i!}. \tag{7}$$

Now, the result of setting $s = -k$, $k = 0, 1, \ldots, r-1$, in (7) and setting $s = c_i$, $i = 1, 2, \ldots, m$ in the first and second derivatives of the polynomials, leads to a linear system for coefficient of the polynomials. The coefficient matrix $A \in \mathbb{R}^{(2m+r)\times(2m+r)}$ is given by

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & \ldots & 0 \\ 1 & \frac{(-1)^1}{1!} & \frac{(-1)^2}{2!} & \frac{(-1)^3}{3!} & \ldots & \frac{(-1)^{2m+r-1}}{(2m+r-1)!} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \frac{(-r+1)^1}{1!} & \frac{(-r+1)^2}{2!} & \frac{(-r+1)^3}{3!} & \ldots & \frac{(-r+1)^{2m+r-1}}{(2m+r-1)!} \\ & & & & & \\ 0 & 1 & \frac{c_1^1}{1!} & \frac{c_1^2}{2!} & \ldots & \frac{c_1^{2m+r-2}}{(2m+r-2)!} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \frac{c_m^1}{1!} & \frac{c_m^2}{2!} & \ldots & \frac{c_m^{2r+m-2}}{(2r+m-2)!} \\ & & & & & \\ 0 & 0 & 1 & \frac{c_1^1}{1!} & \ldots & \frac{c_1^{2m+r-3}}{(2m+r-3)!} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 1 & \frac{c_m^1}{1!} & \ldots & \frac{c_m^{2m+r-3}}{(2m+r-3)!} \end{bmatrix},$$

and the vectors in the right hand of linear system of equations are defined by $\mathbf{u}_r^{[k]} \in \mathbb{R}^r$, $k = 1, 2, \ldots, r$, $\mathbf{v}_m^{[j]} \in \mathbb{R}^m$, $j = 1, 2, \ldots, m$ as

$$(\mathbf{u}_r^{[k]})_i = \begin{cases} 0, & i \neq k, \\ 1, & i = k, \end{cases} \qquad (\mathbf{v}_m^{[j]})_i = \begin{cases} 0, & i \neq j, \\ 1, & i = j. \end{cases}$$

By solving the systems

$$\begin{aligned} A\Phi^{[k]} &= [\mathbf{u}_r^{[k+1]}, \mathbf{0}_m, \mathbf{0}_m]^T, \ k = 0, 1, \ldots, r-1, \\ A\Psi^{[j]} &= [\mathbf{0}_r, \mathbf{v}_m^{[j]}, \mathbf{0}_m]^T, \qquad j = 1, 2, \ldots, m, \\ A\chi^{[j]} &= [\mathbf{0}_r, \mathbf{0}_m, \mathbf{v}_m^{[j]}]^T, \qquad j = 1, 2, \ldots, m, \end{aligned} \tag{8}$$

the coefficients of the polynomials are determined.

Now, the conditions for applying the poising condition [9] are established. Poising condition is a criterion that determines whether the given set of data points can be interpolated using the Hermite–Birkhoff interpolation. By using this condition, it can be shown that the solution of the interpolation problems can be determined uniquely. For this purpose, the following theorems, which are needed to check the uniqueness of the solution of the Hermite–Birkhoff interpolation, are mentioned [9]:

Let k and n be natural numbers, and define the matrix

$$E = \|\epsilon_{ij}\|, \quad i = 1, \ldots, k, \ j = 0, 1, \ldots, n-1,$$

as a matrix with k rows and n columns having elements

$$\epsilon_{ij} = 0 \ \text{ or } \ 1,$$

which are such that

$$\sum_{i,j} \epsilon_{ij} = n.$$

We shall also assume that the matrix E has no zero rows. Also, suppose that $\{x_i\}_{i=1}^k$ is an increasing real number as

$$x_1 < x_2 < \cdots < x_k.$$

Also, the set of ordered pairs is considered by

$$e = \{(i,j) \mid \ \epsilon_{ij} = 1\}.$$

The interpolation problem is described by the reals x_i and the "incidence matrix" E in the form

$$f^{(j)}(x_i) = y_i^{(j)} \quad \text{for} \quad (i,j) \in e. \tag{9}$$

The matrix E has a structure where each row corresponds to a different interpolation point, and the columns represent the derivatives at those points. It is appropriate to see (9) from the point of view of a Hermite–Birkhoff interpolation problem which we show it in an abbreviated form by HB-problem.

Definition 1. When the conditions

$$P(x) \in \pi_{n-1}, \quad P^{(j)}(x_i) = 0, \quad \text{for all } (i,j) \in E,$$

are established, then the HB-problem (9) is poised, and as a result, $P(x) \equiv 0$, equivalently, the matrix E is called poised if the related interpolation problem has a unique solution for any set of constants $y_i^{(j)}$, in which the problem is independent of choosing of the ordered interpolation points $x_l, x_2, \ldots, x_k$.

Define

$$\tilde{m}_j = \sum_{i=1}^{k} \epsilon_{i,j}, \quad \tilde{M}_l = \sum_{j=0}^{l} \tilde{m}_j, \quad j, l = 0, 1, \ldots, n-1.$$

It is shown by Schoenberg [18] that a necessary condition for poising of E is

$$\tilde{M}_l \geq l + 1, \quad l = 0, 1, \ldots, n-1,$$

and these inequalities are recognized as Polya conditions.

Definition 2. Let the incidence matrix E be with k rows. Let f_i be the column index of the first one that appears in the row i. Moreover, E is called a pyramid matrix if, for each i, $\epsilon_{ij} = 1$ implies $\epsilon_{ij'} = 1$ for $f_i \leq j' \leq j$, and there is some value of $1 \leq i \leq k$ so that $f_1 \geq f_2 \geq \cdots \geq f_i$ and $f_i \leq f_{i+1} \leq \cdots \leq f_k$.

The necessary condition for poising the matrix E with respect to the ordering points $x_1 < x_2 < \cdots < x_k$, is declared by Ferguson [9] in the next theorem.

Theorem 1. If E is a pyramid matrix with k rows, satisfying the Polya conditions, then E is poised with respect to the ordering $x_1 < x_2 < \cdots < x_k$.

Now, we show that our interpolation problems (5)–(6) have unique solution or equivalently the conditions hold true for the given interpolation problem. For these problems, the interpolation points can be considered by

$$-r+1 < -r+2 < \cdots < -1 < 0 < c_1 < c_2 < \cdots < c_m.$$

So, the matrix E with $m+r$ rows and $2m+r$ columns can be defined by

$$E = \begin{bmatrix} 1\,0\,0\,0 \cdots 0 \\ 1\,0\,0\,0 \cdots 0 \\ \vdots\;\vdots\;\vdots \qquad \vdots \\ 1\,0\,0\,0 \cdots 0 \\ 0\,1\,1\,0 \cdots 0 \\ \vdots\;\vdots\;\vdots \qquad \vdots \\ 0\,1\,1\,0 \cdots 0 \end{bmatrix}.$$

Thus, we have

$$\tilde{m}_0 = r, \quad \tilde{m}_1 = m, \quad \tilde{m}_2 = m, \quad \tilde{m}_3 = 0, \; \ldots, \tilde{m}_{n-1} = 0,$$

$$\tilde{M}_0 = r, \quad \tilde{M}_1 = r+m, \quad \tilde{M}_3 = 2m+r, \; \ldots, \; \tilde{M}_{n-1} = 2m+r = n.$$

By considering the numbers $\tilde{M}_j$, since

$$\tilde{M}_0 >= 1, \quad \tilde{M}_1 >= 2, \quad \tilde{M}_3 >= 3, \; \ldots, \; \tilde{M}_{n-1} >= n.$$

the Polya condition is satisfied for the matrix E. Also, by considering

$$f_1 = 0, \; f_2 = 0, \; \ldots, \; f_r = 0, \; f_{r+1} = 1, \; \ldots, \; f_{r+m} = 1,$$

according Definition 2, one can see that the matrix E is a pyramid matrix. Thus, by Theorem 1, it is concluded that E is poised with respect to the ordering points $-r+1 < -r+2 < \cdots < -1 < 0 < c_1 < c_2 < \cdots < c_m$. Thus, satisfying these conditions guarantees a unique and smooth interpolating polynomial that satisfies the given data (5)–(6). In the other word, the matrix A is nonsingular.

When a nonlinear ODE is integrated by implicit (first derivative) methods, the approximation of the stage values leads to solving a nonlinear algebraic system of equations, which can be solved by Newton's iterative methods. Thus, the Jacobian matrix $\partial f/\partial y$ is usually computed. Therefore, computing the second derivative function $g := (\partial f/\partial y)f(y)$ does not impose any additional computational cost. It should be mentioned that in the application of these methods, the Jacobian matrix $\partial g/\partial y$ is approximated by $(\partial f/\partial y)^2$, which is a piecewise constant approximation.

3 Continuous order conditions

In this section, we investigate continuous order conditions for the method (2). We know that the collocation polynomial $P(t_n + sh)$ provides a uniform approximation of order p to $y(t_n + sh)$, $s \in [0, 1]$. For this end, the approximate solution $P(t_n + sh)$ is replaced by $y(t_n + sh)$ in (2), where $y(t)$ is the exact solution of (1). Then by subtracting the both sides of the obtained relation, the discretization error is obtained in the form

$$\begin{aligned}\varepsilon(t_n + sh) =& y(t_n + sh) - \sum_{k=0}^{r-1} \varphi_k(s) y(t_{n-k}) - h \sum_{j=1}^{m} \psi_j(s) f(y(t_{n,j})) \\ &- h^2 \sum_{j=1}^{m} \chi_j(s) g(y(t_{n,j})),\end{aligned} \tag{10}$$

where $s \in [0, 1]$ and $n = 1, 2, \ldots, N-1$. By expanding local discretization error in Taylor series around the point t_n and collecting terms with the same powers of h we have the following theorem.

Theorem 2. Assume that the function $f(y)$ is sufficiently smooth. Then the method (2) has uniform order p if the following conditions are satisfied:

$$
\begin{cases}
\displaystyle\sum_{k=0}^{r-1} \varphi_k(s) = 1, \\
\displaystyle\sum_{k=0}^{r-1} k\varphi_k(s) + \sum_{j=1}^{m} \psi_j(s) = s, \\
\displaystyle\sum_{k=0}^{r-1} \frac{(-k)^i}{i!}\varphi_k(s) + \sum_{j=1}^{m} \left(\psi_j(s)\frac{c_j^{i-1}}{(i-1)!} + \chi_j(s)\frac{c_j^{i-2}}{(i-2)!} \right) = \frac{s^i}{i!},
\end{cases} \tag{11}
$$

where $s \in [0,1]$, $i = 2,3,\dots,p$. Moreover, the local discretization error (10) takes the form

$$
\varepsilon(t_n + sh) = h^{p+1} C_p(s) y^{(p+1)}(t_n) + \mathcal{O}(h^{p+2}), \tag{12}
$$

in which

$$
\begin{aligned}
C_p(s) =& \frac{s^{p+1}}{(p+1)!} - \sum_{k=0}^{r-1} \frac{(-k)^{p+1}}{(p+1)!}\varphi_k(s) \\
& - \sum_{j=1}^{m} \left(\psi_j(s)\frac{(c_j)^p}{p!} + \chi_j(s)\frac{c_j^{p-1}}{(p-1)!} \right).
\end{aligned} \tag{13}
$$

The set of order conditions (11) leads to a linear system of $p+1$ equations in $2m+r$ unknowns. The unknowns of this system are the coefficient polynomials of the proposed method.

Therefore, considering p at most equal to $2m+r-1$ guarantees that the linear system (11) is compatible. This leads to the following result.

Remark 1. The maximum attainable uniform order of convergence for the new method (2) is $2m+r-1$.

In the following, the necessary conditions for zero-stability of the new method are investigated. For this end, the method is applied to the simple ODE $y' = 0$, where the recurrence relation is obtained in the form

$$
y_{n+1} = \sum_{k=0}^{r-1} \theta_k y_{n-k},
$$

where $\theta_k = \varphi_k(1)$. Thus, the characteristic polynomial of this recurrence relation is

$$p(\omega) = \sum_{k=0}^{r-1} \theta_k \omega^k,$$

Therefore, the constructed method is zero-stable if and only if $-1 < \theta_i \leq 1$ for $i = 1, 2, \ldots, r-1$.

4 Linear stability analysis

We now focus our attention on the linear stability properties of the SDMCMs (2) with respect to the standard basic test equation of Dahlquist

$$y' = \lambda y, \tag{14}$$

where λ is a complex number with negative real part. Let us consider the vectors and matrices

$$\begin{aligned}
&A = [\psi_j(c_i)]_{i,j=1}^m \in \mathbb{R}^{m\times m}, && \overline{A} = [\chi_j(c_i)]_{i,j=1}^m \in \mathbb{R}^{m\times m},\\
&v^T = [\psi_i(1)]^T \in \mathbb{R}^m, && w^T = [\chi_i(1)]^T \in \mathbb{R}^m,\\
&(\varphi(c))_{j,i} = [\varphi_j(c_i)] \in \mathbb{R}^{m\times r}, && j = 0, 1, \ldots, r-1, \quad i = 1, 2, \ldots, m,\\
&P(t_n + ch) = [P(t_n + c_i h)]_{i,j=1}^m.
\end{aligned} \tag{15}$$

Theorem 3. Applying the new method (2) to the basic test equation (14) leads to the recurrence relation in the form

$$\begin{bmatrix} y_{n+1} \\ y_n^{(r)} \end{bmatrix} = \begin{bmatrix} M_{11}(z) & 0 \\ \mathbf{I}_r & \mathbf{0}_{r,1} \end{bmatrix} \begin{bmatrix} y_n \\ y_{n-1}^{(r)} \end{bmatrix}, \tag{16}$$

where $z := \lambda h$ and

$$\begin{aligned}
&M_{11}(z) = \varphi(1) + \left(z v^T + z^2 w^T\right) Q^{-1} \varphi(c) \in \mathbb{R}^{1\times r},\\
&Q = \mathbf{I}_m - zA - z^2 \overline{A} \in \mathbb{R}^{m\times m}.
\end{aligned}$$

Proof. First, the new constructed method (2) is applied to the test equation (14), and then both sides of the obtained equation are collocated at points $c_i, \quad i = 1, \ldots, m$. Thus the algebraic relation is obtained in the form

$$P(t_n + c_i h) = \sum_{k=0}^{r-1} \varphi_k(c_i) y_{n-k} + \lambda h \sum_{j=1}^{m} \psi_j(c_i) P(t_{n,j}) + \lambda^2 h^2 \sum_{j=1}^{m} \chi_j(c_i) P(t_{n,j}), \tag{17}$$

for $i = 1, \ldots, m$. Also, the approximated solution in the next step is obtained by

$$y_{n+1} = \sum_{k=0}^{r-1} \varphi_k(1) y_{n-k} + \lambda h \sum_{j=1}^{m} \psi_j(1) P(t_{n,j}) + \lambda^2 h^2 \sum_{j=1}^{m} \chi_j(1) P(t_{n,j}), \tag{18}$$

for $n = r-1, r, \ldots, N-1$. By the notations introduced in (15), the relations (17)–(18) can be written in the matrix form as

$$\begin{cases} P(t_n + ch) = \varphi(c)\mathbf{y}_n^{(r)} + zAP(t_n + ch) + z^2 \overline{A} P(t_n + ch), \\ \qquad y_{n+1} = \varphi(1)\mathbf{y}_n^{(r)} + zv^T P(t_n + ch) + z^2 w^T P(t_n + ch). \end{cases} \tag{19}$$

Thus by setting $Q = \mathbf{I} - zA - z^2\overline{A}$, the first relation in (19) leads to

$$P(t_n + ch) = Q^{-1}\varphi(c)\mathbf{y}_n^{(r)},$$

where substituting it in (19) for computing y_{n+1} leads to

$$y_{n+1} = \Big(\varphi(1) + (zv^T + z^2 w^T) Q^{-1} \varphi(c)\Big)\mathbf{y}_n^{(r)}. \tag{20}$$

This relation is equivalent by the first row of (16) and the proof is complete. □

The coefficient matrix in (16) is shown by $R(z) \in \mathbb{C}^{(r+1)\times(r+1)}$, and it is called the stability matrix of the method. So the stability function is obtained by

$$p(\omega, z) = \det(\omega I - R(z)). \tag{21}$$

The stability properties of (2) with respect to the standard test equation (14) are dependent on the corresponding stability function $p(\omega, z)$.

Now, by multiplying the stability function (21) by its denominator, the stability polynomial of the method is obtained, which will be shown by the same symbol $p(w, z)$. Therefore, the stability properties of the corresponding methods depend on the obtained polynomial $p(w, z)$. The region of absolute stability, $\mathcal{A}$, is defined to be a region of the complex z-plane such that the roots of $p(\omega, z) = 0$ lie within the unit circle whenever z lies in the interior of the region. To obtain the region of absolute stability, we use the boundary locus method [15]. Inserting $w = e^{i\theta}$, the roots of stability polynomial describe the bound of stability region.

5 Construction of A-stable SDMCMs

In this section, we focus our attentions on two steps and three steps continuous methods, $(r = 2, 3)$ with one and two collocation parameters. The polynomials of the methods are constructed by solving the linear system (8). Also, one can construct these polynomials by solving the system of order conditions (11) by $p = 2m + r - 1$. Then, by considering the stability matrix (16), collocation parameters in the interval $[0, 1]$ are determined in order to achieve A-stability.

5.1 Construction of SDMCMs with $r = 2$ and $m = 1$

In this subsection, we first investigate two step new methods with $r = 2$ and one collocation parameter of order $p = 2m + r - 1 = 3$. The coefficients of these methods are

$$\varphi_0(s) = \frac{s^3 - 3cs^2 + 3c^2s + 3c^2 + 3c + 1}{3c^2 + 3c + 1},$$

$$\varphi_1(s) = -\frac{s(s^2 - 3cs + 3c^2)}{3c^2 + 3c + 1},$$

$$\psi_1(s) = \frac{(-s^2 + 3cs + 3c + 1)s}{3c^2 + 3c + 1},$$

$$\chi_1(s) = \frac{s((2c + 1)s^2 - (3c^2 + 1)s - 3c^2 - 2c)}{2(3c^2 + 3c + 1)}.$$

The stability polynomial of the method is written in the form

$$p(w, z) = \sum_{i=1}^{3} p_i(z) w^i$$

$$
\begin{aligned}
=&\frac{1}{6c^2+6c+2}\Big(\Big((c^4+2c^3+c^2)z^2+(-4c^3-6c^2-2c)z+6c^2+6c+2\Big)w^3\\
&+\Big((-2c^4+4c^2-2)z^2+(8c^3-8c)z-12c^2-4\Big)w^2\\
&+\Big((c^4-2c^3+c^2)z^2+(-4c^3+6c^2-2c)z+6c^2-6c+2\Big)w\Big).
\end{aligned}
$$

By performing an advanced search based on the boundary locus method, we find that there are some A-stable methods within this class of methods, for example, when the collocation parameter c lies in the interval $[0.578, 1]$, the obtained method is the A-stable of order 3. For example, by choosing $c = 1$, an A-stable method of order 3 is obtained where the polynomials of methods are in the form

$$
\varphi_0(s) = \frac{s^3-3s^2+3s+7}{7}, \quad \varphi_1(s) = \frac{-s^3+3s^2-3s}{7},
$$

$$
\psi_1(s) = \frac{-s^3+3s^2+4s}{7}, \quad \chi_1(s) = \frac{3s^3-2s^2-5s}{14}.
$$

5.2 Construction of SDMCMs with $r = 2$ and $m = 2$

In this subsection, we describe the construction of the method with $r = 2$ and two collocation parameters. The polynomials of method are of degree 5 and can be obtained by solving the system of order condition (11) with $p = 2m + r - 1 = 5$. The stability polynomial of the method is obtained in the form

$$
p(w, z) = \sum_{i=1}^{3} p_i(z) w^i,
$$

where $p_i(z)$ are polynomials of degree 2. By an extensive computer searching, we could not found A-stable methods for $c_1, c_2 \in [0, 1]$, but in some cases, an extensive stability region (near to A-stability) can be observed.

For example, choosing $c = [\frac{1}{2}, 1]$ leads to method of order 5 with unbounded stability region, where its stability region is plotted in Figure 1, and its coefficients are determined by

$$
\varphi_0(s) = 1 + \frac{15}{182}s - \frac{45}{182}s^2 + \frac{5}{14}s^3 - \frac{45}{182}s^4 + \frac{6}{91}s^5,
$$

$$\varphi_1(s) = \frac{-15}{182}s + \frac{45}{182}s^2 - \frac{5}{14}s^3 + \frac{45}{182}s^4 - \frac{6}{91}s^5,$$

$$\psi_1(s) = \frac{-124}{91}s + \frac{372}{91}s^2 - \frac{4}{7}s^3 - \frac{356}{91}s^4 + \frac{192}{91}s^5,$$

$$\psi_2(s) = \frac{415}{182}s - \frac{699}{182}s^2 + \frac{3}{14}s^3 + \frac{757}{182}s^4 - \frac{198}{91}s^5,$$

$$\chi_1(s) = \frac{-209}{182}s + \frac{263}{182}s^2 + \frac{5}{14}s^3 - \frac{283}{182}s^4 + \frac{62}{91}s^5,$$

$$\chi_2(s) = \frac{-149}{364}s + \frac{265}{364}s^2 - \frac{3}{28}s^3 - \frac{281}{364}s^4 + \frac{43}{91}s^5.$$

Also, the stability polynomial of this method is

$$\begin{aligned} p(\omega, z) = \quad & \tfrac{\omega}{2912}(18z^4 - 150z^3 + 727z^2 - 2120z + 2912)\omega^2 \\ & + \tfrac{\omega}{2912}\big((-72z^2 - 768z - 2944)\omega + z^2 + 8z + 32\big). \end{aligned}$$

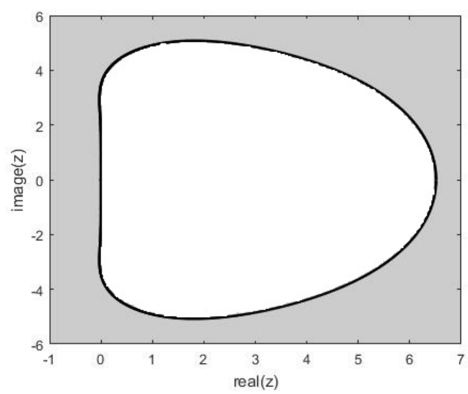

Figure 1: Stability region (Shaded region) of method with $r = 2$, $m = 2$ and $c = [\frac{1}{2}, 1]$.

5.3 Construction of SDMCMs with $r = 3$ and $m = 1$

We now consider 3-step SDMCMs with one collocation parameter of order $p = 4$. Solving the system of order condition (11) corresponding to $p = 4$, we obtain the family of methods of order 4 depending on the parameter c. We apply the boundary locus method on the stability polynomial $p(w, z)$, in order to determine the values of the free parameters $c \in [0,1]$ achieving A-stability. We obtained when c belongs in $[0.619, 1]$, the constructed methods are A-stable. Choosing, for example, for $c = \frac{7}{10}$, we obtain the three-step formula of uniform order $p = 4$ with coefficients given by

$$\varphi_0(s) = 1 + \frac{7}{10}s - \frac{81}{170}s^2 - \frac{11}{170}s^3 + \frac{19}{170}s^4,$$

$$\varphi_1(s) = -\frac{4}{5}s + \frac{42}{85}s^2 + \frac{12}{85}s^3 - \frac{13}{85}s^4,$$

$$\varphi_2(s) = \frac{1}{10}s - \frac{3}{170}s^2 - \frac{13}{170}s^3 + \frac{7}{170}s^4,$$

$$\psi_1(s) = \frac{2}{5}s + \frac{39}{85}s^2 - \frac{1}{85}s^3 - \frac{6}{85}s^4,$$

$$\chi_1(s) = \frac{-1}{5}s - \frac{29}{170}s^2 + \frac{8}{85}s^3 + \frac{11}{170}s^4.$$

5.4 Construction of SDMCMs with $r = 3$ and $m = 2$

We now present the construction for SDMCMs of uniform convergence order 6 with $r = 3$ and $m = 2$. First, by solving the order conditions (11), the polynomials of a method of degree 6 are determined depending on the parameters c_1 and c_2. The stability polynomial of the method is obtained in the form

$$p(w, z) = \sum_{i=1}^{4} p_i(z) w^i,$$

where $p_i(z)$ are polynomials of degree 2. We apply the boundary locus method on the stability polynomial $p(w, z)$, in order to determine the values of the free parameters $c_1, c_2 \in [0,1]$ achieving A-stability. The range of (c_1, c_2) in the domain $[0,1] \times [0,1]$, which leads to A-stable methods, is plotted in Figure 2.

For example, by choosing $c = [\frac{1}{2}, 1]$, an A-stable method of order $p = 6$ is obtained, where coefficients are

$$\varphi_0(s) = \frac{13216s^6 - 21564s^5 - 33123s^4 + 101259s^3 - 87639s^2 + 32517s + 219758}{219758},$$

$$\varphi_1(s) = \frac{-14672s^6 + 25536s^5 + 30786s^4 - 103768s^3 + 91308s^2 - 34104s}{219758},$$

$$\varphi_2(s) = \frac{1456s^6 - 3972s^5 + 2337s^4 + 2509s^3 - 3669s^2 + 1587s}{219758},$$

$$\psi_1(s) = \frac{77504s^6 + 20400s^5 - 305456s^4 + 70768s^3 + 253872s^2 - 65248s}{109879},$$

$$\psi_2(s) = \frac{-83384s^6 - 11604s^5 + 323186s^4 - 120143s^3 - 211887s^2 + 159662s}{109879},$$

$$\chi_1(s) = \frac{2744s^6 - 680s^5 - 11128s^4 + 8296s^3 + 7520s^2 - 8480s}{9989},$$

$$\chi_2(s) = \frac{33320s^6 + 12944s^5 - 116167s^4 + 33872s^3 + 76025s^2 - 53638s}{219758}.$$

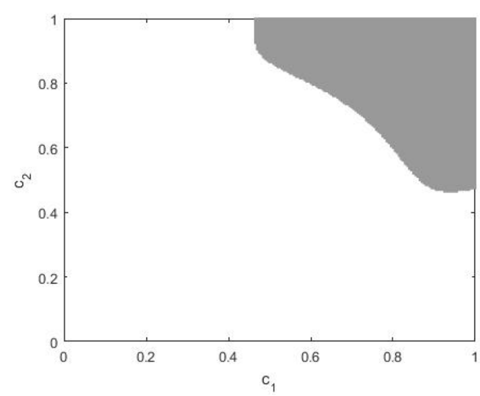

Figure 2: Acceptable (c_1, c_2) pairs for A-stability of SDMCMs with $r = 3,\ m = 2$.

6 Numerical eexperiments

In this section, we present numerical results arising from the application of the SDMCMs in order to confirm the theoretical expectations, show the efficiency and accuracy of the new method, and validate the order of these methods in the integration of stiff systems. In what follows, we describe the details of the implemented methods:

- **Method 1:** A-stable SDMCM of convergence order 3 with $r = 2,\ m = 1$, and collocation parameter $c = 1$.

- **Method 2:** SDMCM of convergence order 5 with $r = 2,\ m = 2$, and collocation parameters $c_1 = \frac{5}{10},\ c_2 = 1$.
- **Method 3:** A-stable SDMCM of convergence order 4 with $r = 3,\ m = 1$, and collocation parameter $c = 1$.
- **Method 4:** A-stable SDMCM of convergence order 6 with $r = 3,\ m = 2$, and collocation parameters $c = [\frac{1}{2}, 1]$.

Also, we compared the results with the method in [6, 8], by the implementation of the method.

- **Method 5:** Second derivative two-step collocation method with $m = 1$, $p = 4m = 4$, $c = \frac{2}{3}$ and $q = 1$, introduced in [8].
- **Method 6:** Two-step almost collocation method with $m = 2$, $p = 2m = 4$, $c = [\frac{1}{2}, \frac{9}{10}]$, introduced in [6].

Computational experiments are done by applying the methods to the following problems:

P1. The nonlinear stiff ODE

$$\begin{cases} y_1'(t) = -10004y_1(t) + 10000y_2(t)^2, \ y_1(0) = 1, \\ y_2'(t) = y_1(t) - y_2(t)(1 + y_2(t)^3), \qquad y_2(0) = 1, \end{cases}$$

with $t \in [0, 1]$. The exact solution is $[y_1(t) \quad y_2(t)]^T = [e^{-4t} \quad e^{-t}]^T$.

P2. The Robertson chemical kinetics problem [13]

$$\begin{cases} y_1'(t) = -0.04y_1(t) + 10^4 y_2(t)y_3(t), & y_1(0) = 1, \\ y_2'(t) = 0.04y_1(t) - 10^4 y_2(t)y_3(t) - 3 \times 10^7 y_2(t)^2, & y_2(0) = 0, \\ y_3' = 3 \times 10^7 y_2(t)^2, & y_3(0) = 0, \end{cases}$$

with $t \in [0, 1000]$.

P3. The Pleiades problem [16] is a celestial mechanics problem of seven stars in the plane of coordinates x_i and y_i and masses $m_i = i$ for $i = 1, 2, \ldots, 7$. The problem consists of a system of 14 special second-order differential equations rewritten to a first-order form, thus providing a system of ODEs of dimension 28. The formulation and data have been taken from [11]. The problem is in the form

$$z'' = f(z), \quad z(0) = z_0, \quad z'(0) = z_0',$$

with $z \in \mathbb{R}^{14}$ and $0 \leq t \leq 3$. By considering $z = (x^T, y^T)^T$, $x, y \in \mathbb{R}^7$, the function $f : \mathbb{R}^{14} \to \mathbb{R}^{14}$ is given by $f(z) = f(x, y) = (f^{(1)}(x, y), f^{(2)}(x, y))^T$, where $f^{(1)}, f^{(2)} : \mathbb{R}^{14} \to \mathbb{R}^7$ are

$$\begin{aligned} f_i^{(1)} &= \sum_{j \neq i} m_j (x_j - x_i)/r_{ij}^{3/2}, \\ f_i^{(2)} &= \sum_{j \neq i} m_j (y_j - y_i)/r_{ij}^{3/2}, \quad i = 1, 2, \ldots, 7, \end{aligned}$$

with $m_i = i$ and

$$r_{i,j} = (x_i - x_j)^2 + (y_i - y_j)^2.$$

We convert this problem to a first-order form by defining $w = z'$, which leads to a system of 28 nonlinear differential equations of the form

$$\begin{pmatrix} z' \\ w' \end{pmatrix} = \begin{pmatrix} w \\ f(z) \end{pmatrix},$$

where $(z^T, w^T)^T \in \mathbb{R}^{28}$ and $0 \leq t \leq 3$. The initial values are

$$\begin{pmatrix} z_0 \\ w_0 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \\ x_0' \\ y_0' \end{pmatrix}, \quad \begin{cases} x_0 = (3, 3, -1, -3, 2, -2, 2)^T, \\ y_0 = (3, -3, 2, 0, 0, -4, 4)^T, \\ x_0' = (0, 0, 0, 0, 0, 1.75, -1, 5)^T, \\ y_0' = (0, 0, 0, -1.25, 1, 0, 0)^T. \end{cases}$$

Table 1 presents the reference solution at the end of the integration interval, which is reported in [16].

In our numerical experiments, we apply Method 1– Method 4 to the given test problems with the fixed step sizes $h = T/N$ for several integer values of N. The global error of the methods at the endpoint of the interval of integration is listed by Err. Also, to verify theoretical results on the order of accuracy, we compute a numerical estimate to the order of accuracy of the methods by the formula $\log_2(\|Err_h(x)\|/\|Err_{h/2}(x)\|)$, where $Err_h(x)$ and $Err_{h/2}(x)$

Table 1: Reference solution at the end of the integration interval

x_1 =0.3706139143970502	y_1 = -3.943437585517392
x_2 = 3.237284092057233	y_2 = -3.271380973972550
x_3 = -3.222559032418324	y_3 =5.225081843456543
x_4 = 0.6597091455775310	y_4 =-2.590612434977470
x_5 = 0.3425581707156584	y_5 = 1.198213693392275
x_6=1.562172101400631	y_6 = -0.2429682344935824
x_7 = -0.7003092922212495	y_7 = 1.091449240428980
$x'_1 = 3.417003806314313$	$y'_1 = -3.741244961234010$
$x'_2 = 1.354584501625501$	$y'_2 = 0.3773459685750630$
$x'_3 = -2.590065597810775$	$y'_3 = 0.9386858869551073$
$x'_4 = 2.025053734714242$	$y'_4 = 0.3667922227200571$
$x'_5 = -1.155815100160448$	$y'_5 = -0.3474046353808490$
$x'_6 = -0.8072988170223021$	$y'_6 = 2.344915448180937$
$x'_7 = 0.5952396354208710$	$y'_7 = -1.947020434263292$

are the errors at the endpoint of the interval of integration corresponding to the step sizes h and $h/2$, respectively. we observed that the expected order was achieved. Also, by comparing results by methods introduced in [6, 8], one can see that the results are compatible with Method 5 and the solution by this new method is more precise than the results of Method 4 while the computational cost for the new method is less.

In problems P2, the reference solutions reported in [10] are used for computing the global error. The obtained results are reported in Table 2.

Table 2: The results of the methods for problem **P1**.

	N	4	8	16	32	64
Method 1	Err	2.22×10^{-4}	3.40×10^{-5}	4.64×10^{-6}	6.04×10^{-7}	7.71×10^{-8}
	$p(h)$		2.71	2.87	2.94	2.97
Method 2	Err	2.12×10^{-7}	8.38×10^{-9}	2.93×10^{-10}	9.66×10^{-12}	3.10×10^{-13}
	$p(h)$		4.66	4.84	4.92	4.96
Method 3	Err	1.95×10^{-5}	1.92×10^{-6}	1.39×10^{-7}	9.30×10^{-9}	5.99×10^{-10}
	$p(h)$		3.35	3.78	3.91	3.96
Method 4	Err	3.96×10^{-9}	1.01×10^{-10}	1.93×10^{-12}	3.33×10^{-14}	5.46×10^{-16}
	$p(h)$		5.31	5.70	5.86	5.93
Method 5	Err	1.17×10^{-3}	6.14×10^{-5}	2.58×10^{-6}	1.01×10^{-7}	5.96×10^{-9}
	$p(h)$		4.26	4.57	4.67	4.59
Method 6	Err	1.51×10^{-3}	1.74×10^{-4}	1.49×10^{-5}	1.08×10^{-6}	7.08×10^{-8}
	$p(h)$		3.11	3.54	3.79	3.93

Table 3: The results of SDMCMs for problem **P2**

	N	500	750	1000	1250	1500
Method 1	Err	4.41×10^{-5}	1.69×10^{-6}	8.22×10^{-6}	4.62×10^{-6}	2.85×10^{-7}
	$p(h)$		2.37	2.50	2.58	2.69
Method 2	Err	3.41×10^{-7}	7.41×10^{-8}	2.17×10^{-8}	8.07×10^{-9}	4.46×10^{-9}
	$p(h)$		3.76	4.27	4.42	4.64
Method 3	Err	1.99×10^{-6}	8.24×10^{-7}	3.99×10^{-7}	2.16×10^{-7}	7.81×10^{-8}
	$p(h)$		3.07	3.25	3.36	3.54
Method 4	Err	7.86×10^{-8}	1.67×10^{-8}	5.26×10^{-9}	1.58×10^{-9}	5.42×10^{-10}
	$p(h)$		4.84	4.97	5.37	5.90

Table 4: The results of SDMCMs for problem **P3**

	h	$\frac{1}{2} \times 10^{-3}$	$\frac{1}{4} \times 10^{-3}$	$\frac{1}{8} \times 10^{-3}$	$\frac{1}{16} \times 10^{-3}$
Method 1	Err	1.99×10^{-1}	2.49×10^{-2}	3.13×10^{-3}	3.90×10^{-4}
	$p(h)$		2.99	2.99	3.00
Method 2	Err	7.32×10^{-4}	2.31×10^{-5}	7.21×10^{-7}	2.47×10^{-8}
	$p(h)$		4.98	4.99	5.00
Method 3	Err	5.39×10^{-2}	2.52×10^{-3}	1.24×10^{-4}	6.67×10^{-4}
	$p(h)$		4.41	4.34	4.22
Method 4	Err	2.15×10^{-5}	3.71×10^{-7}	6.02×10^{-9}	9.46×10^{-11}
	$p(h)$		5.86	5.94	5.99

7 Conclusion

We have introduced a new family of SDMCMs. The constructed r-step method with m collocation parameters has a uniform order $2m + r - 1$. Examples of SDMCMs up to order 6 with the property of A-stability were constructed. The accuracy and efficiency of constructed methods were verified by solving some stiff problems. SDMCMs are efficient in solving stiff problems, which are confirmed by numerical experiments. Future work will be in the investigation of G-simplecticity of SDMCMs [12, 17].

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