Earthline Journal of Mathematical Sciences
E-ISSN: 2581-8147
Volume 15, Number 4, 2025, Pages 583-603
https://doi.org/10.34198/ejms.15425.583603

Second Derivative Mono-Implicit Runge-Kutta Methods

A. G. Ariwayo[1], P. O. Olatunji[2,*] and R. I. Okuonghae[3]

[1] Department of Mathematical Sciences, Adekunle Ajasin University, P.M.B 001, Akungba Akoko, Ondo State, Nigeria

[2] Department of Mathematical Sciences, Adekunle Ajasin University, P.M.B 001, Akungba Akoko, Ondo State, Nigeria
e-mail: peter.olatunji@aaua.edu.ng

[3] Advanced Research Laboratory, Department of Mathematics, University of Benin, P.M.B 1154, Benin City, Nigeria

Abstract

Mono-implicit Runge-Kutta (MIRK) methods are Runge-Kutta methods having its stages depending on its output. In this paper, we develop a family of second derivative mono-implicit Runge-Kutta (SDMIRK) methods for the numerical solution of stiff initial value problems (IVPs) in ordinary differential equations (ODEs). The SDMIRK methods are extension of the MIRK having first and second derivative terms. The general order conditions for the stages and output methods are presented. The SDMIRK methods for stages $s = 3$ and $s = 4$ derived were found to be A-stable, while methods for $s = 5$ and $s = 6$ are $A(\alpha)$-stable. Implementation procedures and numerical experiment are discussed herein. Results obtained by the SDMIRK method are favourable than the results of second derivative backward difference formular (SDBDF) and second derivative linear multistep method (SDLMM).

1 Introduction

The modelling of physical phenomena often occur in science, engineering and economics, with some of their applications including the determination of motion of planetary bodies, rate of decay of radioactive elements and change in population over a period of time [5]. These mathematical models always give birth to differential equations that contain some derivatives of unknown function with respect to independent variables. If a differential equation involves a derivative with respect to a single dependent variable, it is called an ordinary differential equation (ODE). Here, our focus is on a subclass of implicit Runge-Kutta (IRK) method called mono-implicit Runge-Kutta (MIRK) method [7] for the numerical solution of stiff initial value problems (IVPs) of ODEs in the form

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

where $y \in \mathbb{R}^m$ and $f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$.

Received: March 17, 2025; Accepted: April 23, 2025; Published: May 1, 2025
2020 Mathematics Subject Classification: 65L05, 65L06.
Keywords and phrases: Runge-Kutta methods, mono-implicit Runge-Kutta methods, order, stiff problems, $A-$, $A(\alpha)-$stability, boundary locus.
*Corresponding author

Runge-Kutta method (RKM) was first proposed by Carl Runge in 1895, further contributions were made by Heun and Martin in 1900 and 1901 respectively [10]. Most explicit RKMs have small region of absolute stability, it is generally known that $4th$ order explicit RKM have a region of stability which intersects the imaginary and the negative real axis at $|h\lambda| \approx 2.7$ [12, 28]. This stability limitation can be resolved by considering IRK integrators. Ehle [19] revealed that the s-stage implicit RKMs derived by Butcher [6, 7] are all A-stable in the spirit of Dahlquist [16]. One practical disadvantage such methods suffer is that, the solution of the non-linear implicit equations occurring at each time step is harder to achieve than in the case of linear multistep methods. Cash [12] constructed efficient L-stable IRK methods similar in design to the classical RKMs suitable for integration of both stiff and non-stiff systems of inherently stable ODEs. The IRK methods derived in [12] have reasonable order accuracy while still maintaining computational accuracy, and preserving the one-step nature of the methods. Voss and Muir [42] revealed that the implicit Runge-Kutta methods suffer from the phenomena of order reduction when applied for the integration of stiff ODEs; regardless of its classical order, the output method will behave as if its order is that of its stage order. Chen [15] proposed IRK methods that prevent the methods from behaving as if they of lower order (i.e suffering from order reduction) by extending the tableau of different types of IRK methods to obtain methods with higher stage order. Okuonghae and Ikhile [37] considered the extension of popular Runge-Kutta method to second derivative IRK methods for the direct solution of stiff initial value ordinary differential equations. The use of collocation and interpolation technique was used for the derivation of these methods. The last stage of the input approximation is identical to the output method, and the methods examined are $L(\alpha)-$stable. Several researchers have also developed IRK methods for stiff IVPs of ODEs include [2–5, 7–10, 12, 18, 21–24, 26, 29, 31, 34, 35, 40, 41, 50–53] just to mention a few. RKMs have also been extended to two-step RKMs (see [43–45]) and second derivative TSRK methods (see [43]). The extension and formation of Runge-Kutta methods has given wider popularity to the RKMs. The general form of an $s-$stage RKM is

$$
\begin{aligned}
Y_r &= y_n + h\sum_{j=1}^{s} a_{r,j} f(k_j), \quad r = 1(1)s, \\
y_{n+1} &= y_n + h\sum_{r=1}^{s} b_r f(Y_r),
\end{aligned} \tag{2}
$$

where h is the step size, s is the number of stages, $Y_r,\ r = 1(1)s$ are the stages and the numerical approximation to the exact solution $y(x_n + c_r h)$, y_{n+1} is the output method and approximation to the exact solution $y(x_n + h)$, and $b_r\ a_{r,j}$ are real and constant coefficients.

The RKM (2) can be represented in Butcher's tableau defined as

$$
\begin{array}{c|c}
c & A \\
\hline
 & b^T
\end{array}
$$

where $A = \{a_{r,j}\}_{r,j=1}^{s}$, $c = (c_1, c_2..., c_s)^T$, $b^T = (b_1, b_2..., b_s)$.

1.1 The Mono Implicit Runge-Kutta Methods

Among the various sub-classes of implicit Runge-Kutta methods (IRK) been proposed for the numerical solution of stiff ODEs is mono-implicit Runge-Kutta (MIRK) method ([13, 14, 18, 30]. Capper and Moore [11] proposed MIRK methods of orders 10 and 12 alongside their the local truncation error, numerical experiments were conducted on some test problems and it was found that the order 12 scheme provides a significantly greater accuracy than the tenth order scheme. Also, [17] investigated the conditions to be met by MIRK methods in order to generate a mono-implicit Runge-Kutta-Nystrom (MIRKN) method that is P-stable. [32] considered MIRKN methods that are suitable for systems of second order ODEs and also derived optimal symmetric methods of orders 2, 4 and 6. [38] introduced continuous MIRKN methods which allows continuous solution and derivative approximation. Most MIRK methods do suffer order reduction (a condition where a numerical scheme converges with numerical order lower than its theoretical order), therefore [18] proposed a generalization of MIRK methods that do not suffer order reduction when applied for the numerical solution of stiff ODEs. The general form of a MIRK method is defined as

$$\begin{aligned} Y_r &= (1 - v_r)y_n + v_r y_{n+1} + h\sum_{j=1}^{r-1} x_{r,j} f(Y_j), \quad r = 1, ..., s, \\ y_{n+1} &= y_n + h\sum_{r=1}^{s} b_r f(Y_r), \end{aligned} \tag{3}$$

where h is the step size, s is the number of stages, Y_r, $r = 1(1)s$ are the stages and the numerical approximation to the exact solution $y(x_n + c_r h)$, y_{n+1} is the output method and approximation to the exact solution $y(x_n + h)$, and b_r $x_{r,j}$ are real and constant coefficients. The MIRK method (3) can be represented in a tableau given as

$$\begin{array}{c|c|c} c & v & X \\ \hline & & b^T \end{array} = \begin{array}{c|c|cccc} c_1 & v_1 & 0 & 0 & \cdots & 0 \\ c_2 & v_2 & a_{21} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_s & v_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\ \hline & & b_1 & b_2 & \cdots & b_s \end{array}, \tag{4}$$

where $v = (v_1, v_2, ..., v_s)^T$, $c = v + Xe = (c_1, c_2, ..., c_s)^T$ and X is s by s matrix whose $(r, j)th$ component is $x_{r,j}$. X is strictly lower triangular matrix. The MIRK method (3) is equivalent to the implicit Runge-Kutta (IRK) (2) with $A = X + vb^T$ [12].

The stability function, $R(z)$, of the MIRK method (4) [15,35] is given by

$$\frac{\bar{P}(z, e-v)}{\bar{P}(z, -v)}, \tag{5}$$

where

$$\bar{P}(z, \bar{u}) = 1 + zb^T(I - zX)^{-1}\bar{u}, \qquad \bar{u} \in \mathbb{R}^s.$$

The stability function is used to determine the stability properties of a MIRK method.

Definition 1.1. The MIRK method (3) is $A-$stable if $|R(z)| \leq 1$, whenever $Re(z) \leq 0$.

Definition 1.2. The MIRK method (3) is $L-$stable if it is $A-$stable and $|R(z)| \to 0$ as $z \to \infty$.

IRK methods that satisfy Definitions 1 and 2 are suitable for the numerical solution of stiff problems (1) [46,47]. The advantage of MIRK methods (3) is that in implementation, it attract low computational cost in term of the number of non-linear equations to be solved. The other sections of this paper are arranged as follows; Section 2 introduces the generalization to the second derivative mono-implicit Runge-Kutta (SDMIRK) methods, Section 3 presents the order conditions and linear stability of the SDMIRK methods, while in Section 4 examples of the SDMIRK methods are derived and numerical experiments are carried out in Section 5.

2 Generalized SDMIRK Methods

Several authors have extended classical numerical methods (which includes, Runge-Kutta methods, linear multistep methods and general linear methods) to second derivative methods, some of which are the works of [23, 29, 31, 33–37, 39, 43, 47–49]. In the same spirit, the MIRK (3) is extended to SDMIRK methods. The proposed generalized SDMIRK scheme for the numerical integration of (1) is given as:

$$\begin{aligned} Y_r &= (1 - v_r)y_n + v_r y_{n+1} + h\sum_{j=1}^{r-1} x_{rj} f(Y_j) + h^2 \sum_{j=1}^{r-1} \bar{x}_{rj} g(Y_r), \qquad r = 1(1)s, \\ y_{n+1} &= y_n + h\sum_{r=1}^{s} b_r f(Y_r) + h^2 \sum_{r=1}^{s} \bar{b}_r g(Y_r), \end{aligned} \tag{6}$$

where h is the step size, s is the number of stages, Y_r, $r = 1(1)s$ are the stages and the numerical approximation to the exact solution $y(x_n + c_r h)$, y_{n+1} is the output method and approximation to the exact solution $y(x_n + h)$, $f(Y_j) \approx y'(x_n + jh)$, $g(Y_j) \approx y''(x_n + jh)$ and $b_r, \bar{b}_r, x_{r,j}, \bar{x}_{r,j}$ are real and constant coefficients. The abscissa $c_r = v_r + \sum_{i=1}^{r-1} x_{ri} + \sum_{i=1}^{r-1} \bar{x}_{ri}$ which is equivalent to $c = Xe + \bar{X}e + v$ in matrix form. The SDMIRK method (6) can also be written in the Butcher's tableau as

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b^T & \bar{b}^T \end{array} = \begin{array}{c|c|ccc|ccc} c_1 & v_1 & x_{11} & \cdots & x_{1s} & \bar{x}_{11} & \cdots & \bar{x}_{1s} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ c_s & v_s & x_{s1} & \cdots & x_{ss} & \bar{x}_{s1} & \cdots & \bar{x}_{ss} \\ \hline & & b_1 & \cdots & b_s & \bar{b}_1 & \cdots & \bar{b}_s \end{array}. \tag{7}$$

In this paper, the coefficients of the SDMIRK method (6) shall be presented in the tableau format (7).

3 Order Conditions and Stability of the SDMIRK Method (6)

The stages $Y_r,\ r = 1(1)s$ of the SDMIRK method (6) are of order q, and it is given by,

$$Y_r = y(x_n + c_r h) + O(h^{q+1}), \qquad r = 1(1)s, \tag{8}$$

and the output method y_{n+1} is of order p, and it is given by,

$$y_{n+1} = y(x_n + h) + O(h^{p+1}). \tag{9}$$

It is therefore possible to derive the stage order conditions and the order order conditions by expanding (11) and (12) by Taylor series about x_n, we therefore state the following theorem.

Theorem 3.1. *The stage Y_r of the SDMIRK method (6) is of order q if*

$$\begin{aligned} &Xe + e = c, && j = 1, \qquad e = (1, 1..., 1)^T, \\ &\frac{Xc^{j-1}}{(j-1)!} + \frac{\bar{X}c^{j-2}}{(j-2)!} + \frac{v}{j!} = \frac{c^j}{j!} && j = 2, 3, ..., q, \end{aligned} \tag{10}$$

and the error constant C_{q+1} of the stage Y_r is

$$C_{q+1} = \frac{c^{q+1}}{(q+1)!} - \left(\frac{Xc^q}{q!} + \frac{\bar{X}c^{q-1}}{(q-1)!} + \frac{v}{(q+1)!} \right), \quad q \geq 1. \tag{11}$$

Proof. For the stages of the SDMIRK method (6), the local truncation error (lte) is given as

$$lte(x_n) = y(x_n + ch) - \big((e - v)y(x_n) + vy(x_n + h) + hXy'(x_n + ch) + h^2\bar{X}y''(x_n + ch)\big) \tag{12}$$

expanding (12) by Taylor's series about x_n gives

$$\begin{aligned} lte(x_n) &= C_0 y(x_n) + C_1 hy'(x_n) + C_2 h^2 y''(x_n) + \cdots + C_q h^q y^{(q)}(x_n) + C_{q+1} h^{q+1} y^{(q+1)}(x_n) + O(h^{q+2}) \\ &\leq C_{q+1} h^{q+1} y^{(q+1)}(x_n) + O(h^{q+2}). \end{aligned} \tag{13}$$

where

$$\begin{gathered} C_0 = 0, \\ C_1 = c - (Xe + e), \\ C_2 = \tfrac{c^2}{2!} - \left(Xc + \bar{X} + \tfrac{v}{2!}\right), \\ \vdots \\ C_q = \tfrac{c^q}{q!} - \left(\tfrac{Xc^{q-1}}{(q-1)!} + \tfrac{\bar{X}c^{q-2}}{(q-2)!} + \tfrac{v}{q!}\right), \\ C_{q+1} = \tfrac{c^{q+1}}{(q+1)!} - \left(\tfrac{Xc^q}{q!} + \tfrac{\bar{X}c^{q-1}}{(q-1)!} + \tfrac{v}{(q+1)!}\right). \end{gathered}$$

Since the method is of order q, then

$$C_0 = C_1 = \cdots = C_q = 0,$$

and $C_{q+1} \neq 0$. Thus giving the order conditions (10) and error constant (11). □

Theorem 3.2. *The output method of the SDMIRK method (6) is of order p if*

$$\begin{aligned} &b^T e = 1, && j = 1, \quad e = (1, 1..., 1)^T, \\ &\frac{b^T c^{j-1}}{(j-1)!} + \frac{\bar{b}^T c^{j-2}}{(j-2)!} = \frac{1}{j!}, && j = 2, 3, ..., p. \end{aligned} \tag{14}$$

and the error constant C_{p+1} of the output method is

$$C_{p+1} = \frac{1}{(p+1)!} - \left(\frac{b^T c^p}{p!} + \frac{\bar{b}^T c^{p-1}}{(p-1)!}\right), \qquad p \geq 1. \tag{15}$$

Proof. For the output method of the SDMIRK method (6), the local truncation error (lte) is given as

$$lte(x_n) = y(x_n + h) - \left(y(x_n) + hb^T y'(x_n + ch) + h^2 \bar{b}^T y''(x_n + ch)\right), \tag{16}$$

again, expanding (16) by Taylor's series about x_n gives

$$\begin{aligned} lte(x_n) &= C_0 y(x_n) + C_1 hy'(x_n) + C_2 h^2 y''(x_n) + \cdots + C_p h^p y^{(p)}(x_n) + C_{p+1} h^{p+1} y^{(p+1)}(x_n) + O(h^{p+2}) \\ &\leq C_{p+1} h^{p+1} y^{(p+1)}(x_n) + O(h^{p+2}). \end{aligned} \tag{17}$$

where

$$\begin{gathered} C_0 = 0, \\ C_1 = 1 - b^T e, \\ C_2 = \tfrac{1}{2!} - \left(b^T c + \bar{b}^T\right), \\ \vdots \\ C_p = \tfrac{1}{p!} - \left(\tfrac{b^T c^{p-1}}{(p-1)!} + \tfrac{\bar{b}^T c^{p-2}}{(p-2)!}\right), \\ C_{p+1} = \tfrac{1}{(p+1)!} - \left(\tfrac{b^T c^p}{p!} + \tfrac{\bar{b}^T c^{p-1}}{(p-1)!}\right). \end{gathered}$$

The output method is of order p, then

$$C_0 = C_1 = \cdots = C_p = 0,$$

however, $C_{p+1} \neq 0$. Thus giving the order conditions (14) and error constant (15). □

Definition 3.3. The SDMIRK method (6) is pre-consistent if

$$\begin{aligned} Xe + v &= c, \\ b^T e &= 1. \end{aligned} \tag{18}$$

Definition 3.4. The SDMIRK method (6) is consistent if $p \geq 1$.

Applying the SDMIRK method (6) written in the tableau form (7) to the scalar test problem,

$$y'(x) = \lambda y(x), \qquad \lambda > 0, \tag{19}$$

we have

$$y_{n+1} = R(z) y_n, \tag{20}$$

where,

$$R(z) = \frac{\bar{P}(z, e - v)}{\bar{P}(z, -v)}, \tag{21}$$

with the definition that

$$\bar{P}(z, w) = 1 + (zb^T + z^2 \bar{b}^T)(I - zX - z^2 \bar{X})^{-1} w. \tag{22}$$

The $R(z)$ in (19) is the stability function of the SDMIRK method (6).

Definition 3.5. The SDMIRK method (6) is $A-$stable if $R(z)$ defined by (17) satisfies $|R(z)| \leq 1$, whenever $Re(z) \leq 0$.

Definition 3.6. The SDMIRK method (6) is $L-$stable if it is $A-$stable and $R(z)$ defined by (17) satisfies $|R(z)| \to 0$ as $z \to \infty$.

In the next section, we construct SDMIRK methods with $s = 3, 4, 5, 6$. These methods are derived in a way that the stage order q equals the output order p. This is to ensure that the SDMIRK methods do not suffer order reduction [see 43].

4 Derivation of the Methods

In the derivation of the SDMIRK method (6) with stage number s and of order $q = p$, the procedures are:

i. choose values for s, q and p. Here, we choose $q = p$.

ii. set the values of s, q and p into the order conditions (10) and (13) for the stages and output method respectively.

iii. obtain the arising system of equations.

iv. solve the arising system of equations in terms of the unknown real constant coefficients $v, b_r, \bar{b}_r, x_{r,j}, \bar{x}_{r,j}$.

v. set values for the abscissae $c_r,\ r = 1(1)s$. Here, the c_r values are chosen as $c_1 = 0,\ c_2 = 1$, and $c_r \neq c_1,\ r = 3(1)s,\ c_r \neq c_2,\ r = 3(1)s$.

Here are some examples of SDMIRK method (6).

4.1 Method of order $p = q = 6$; $s = 3$

Following the approach discussed above, the stage order conditions for the SDMIRK method (6) with $s = 3, p = q = 6$ are given as

$$\begin{gathered} Xe + v = c, \quad Xc + \bar{X}e + \frac{v}{2} = \frac{c^2}{2}, \quad \frac{Xc^2}{2} + \bar{X}c + \frac{v}{6} = \frac{c^3}{5}, \quad \frac{Xc^3}{6} + \frac{\bar{X}c^2}{2} + \frac{v}{24} = \frac{c^4}{24}, \\ \frac{Xc^4}{24} + \frac{\bar{X}c^3}{6} + \frac{v}{120} = \frac{c^5}{120}, \quad \frac{Xc^5}{120} + \frac{\bar{X}c^4}{24} + \frac{v}{720} = \frac{c^6}{720}, \end{gathered} \tag{23}$$

and the output method order conditions are

$$\begin{gathered} b^T e = 1, \quad b^T c + \bar{b}^T e = \frac{1}{2}, \quad b^T c^2 + 2\bar{b}^T c = \frac{1}{3}, \quad b^T c^3 + 3\bar{b}^T c^2 = \frac{1}{4} \\ b^T c^4 + 4\bar{b}^T c^3 = \frac{1}{5}, \quad b^T c^5 + 5\bar{b}^T c^4 = \frac{1}{6}. \end{gathered} \tag{24}$$

Next we solve the system of equations (21) and (22) in terms of $v, X, \bar{X}, b$ and $\bar{b}$ and choose values for the abscissae c. Here, $c_1 = 0,\ c_2 = 1$ and $c_3 \neq 0, 1$. Choosing $c_3 = \frac{4}{5}$, the SDMIRK method (6) with $s = 3, p = q = 6$ is given in the tableau form as

$$\begin{array}{c|c|cc} c & v & X & \bar{X} \\ \hline & & b^T & \bar{b}^T \end{array} = \begin{array}{c|c|ccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{4}{5} & \frac{4303125}{13312} & \frac{-3879865}{26625} & \frac{-4640625}{26624} & \frac{55}{104} & \frac{-1098075}{53248} & \frac{2041875}{53248} & 0 \\ \hline & & \frac{46609}{101250} & \frac{4297}{7986} & \frac{107648}{67381875} & \frac{901}{13500} & \frac{-797}{7260} & \frac{-416}{408375} \end{array}. \tag{25}$$

The stability function of the SDMIRK method (23) is

$$R(z) = \frac{5760 - 3560z - 468z^2 + 462z^3 + 121z^4}{3(1920 - 3040z + 1924z^2 - 570z^3 + 75z^4)}.$$

The boundary locus plot of the SDMIRK method (23) is shown in Figure 1. The stability plot shows that the SDMIRK method (23) is $A-$stable (since the stability lies in the entire left half of the complex plane).

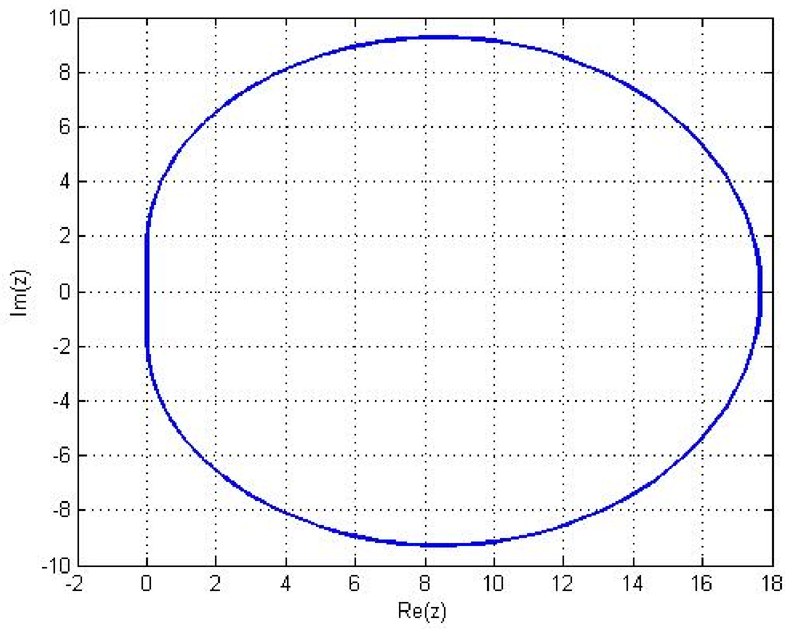

Figure 1: Boundary locus plot of the SDMIRK method (23).

4.2 Method of order $p = q = 7$; $s = 4$

The stage order conditions of the SDMIRK method (6) with $s = 4$, $p = q = 7$ are given as

$$
\begin{aligned}
&Xe + v = c, \quad Xc + \bar{X}e + \frac{v}{2} = \frac{c^2}{2}, \quad \frac{Xc^2}{2} + \bar{X}c + \frac{v}{6} = \frac{c^3}{6}, \quad \frac{Xc^3}{6} + \frac{\bar{X}c^2}{2} + \frac{v}{24} = \frac{c^4}{24}, \\
&\frac{Xc^4}{24} + \frac{\bar{X}c^3}{6} + \frac{v}{120} = \frac{c^5}{120}, \quad \frac{Xc^5}{120} + \frac{\bar{X}c^4}{24} + \frac{v}{720} = \frac{c^6}{720}, \quad \frac{Xc^6}{720} + \frac{\bar{X}c^5}{120} + \frac{v}{5040} = \frac{c^7}{5040},
\end{aligned} \tag{26}
$$

and the output method order conditions are

$$
\begin{aligned}
&b^T e = 1, \quad b^T c + \bar{b}^T e = \frac{1}{2}, \quad \frac{1}{2}b^T c^2 + \bar{b}^T c = \frac{1}{6}, \quad \frac{1}{6}b^T c^3 + \frac{1}{2}\bar{b}^T c^2 = \frac{1}{24}, \\
&\frac{1}{24}b^T c^4 + \frac{1}{6}\bar{b}^T c^3 = \frac{1}{120}, \quad \frac{1}{120}b^T c^5 + \frac{1}{24}\bar{b}^T c^4 = \frac{1}{720}, \quad \frac{1}{720}b^T c^6 + \frac{1}{120}\bar{b}^T c^5 = \frac{1}{5040}.
\end{aligned} \tag{27}
$$

Solving the systems of equations (24) and (25), then setting $c = (0, 1, \frac{1}{2}, \frac{3}{4})^T$ gives the SDMIRK method (6) of order $p = q = 7$ for $s = 4$ defined by

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b^T & \bar{b}^T \end{array} = \begin{array}{c|c|cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & \frac{3}{32} & \frac{-3}{32} & 0 & 0 & \frac{1}{192} & \frac{1}{192} & \frac{-1}{24} & 0 \\ \frac{3}{4} & \frac{1431}{2048} & \frac{237}{4096} & \frac{-459}{4096} & \frac{27}{250} & 0 & \frac{27}{8192} & \frac{45}{8192} & \frac{-9}{512} & 0 \\ \hline & & 0 & \frac{251}{91} & \frac{-544}{91} & \frac{384}{91} & \frac{-46}{4095} & \frac{-523}{2730} & \frac{-1163}{1365} & \frac{-5648}{4095} \end{array}, \qquad (28)$$

with the stability function given as

$$R(z) = \frac{16773120 - 28811520z - 15177120z^2 - 3221040z^3 - 381468z^4 - 27118z^5 - 1059z^6}{16773120 - 45584640z + 22020960z^2 - 5245200z^3 + 751812z^4 - 66906z^5 + 3177z^6}.$$

The boundary locus plot of the SDMIRK method (26) is shown in Figure 2, and it is seen that the SDMIRK method (26) is $A-$stable. (having the region of absolute stability in the interval $(-\infty, 0]$).

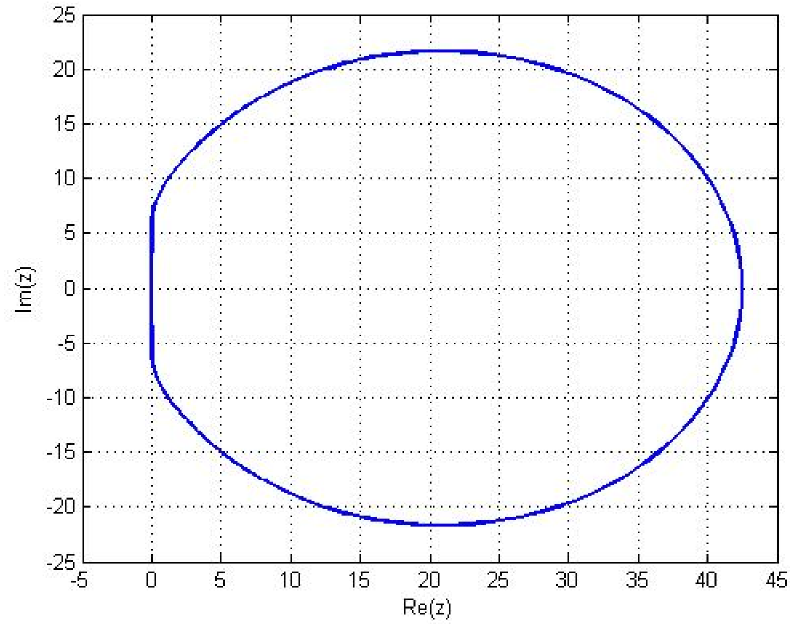

Figure 2: Boundary locus plot of the SDMIRK method (26).

4.3 Method of order $p = q = 9$; $s = 5$

The stage order conditions for the SDMIRK method (6) with $s = 5$ and order $p = q = 9$ are given as

$$\begin{gathered} Xe + v = c, \quad Xc + \bar{X}e + \frac{v}{2} = \frac{c^2}{2}, \quad \frac{Xc^2}{2} + \bar{X}c + \frac{v}{6} = \frac{c^3}{6}, \quad \frac{Xc^3}{6} + \frac{\bar{X}c^2}{2} + \frac{v}{24} = \frac{c^4}{24}, \\ \frac{Xc^4}{24} + \frac{\bar{X}c^3}{6} + \frac{v}{120} = \frac{c^5}{120}, \quad \frac{Xc^5}{120} + \frac{\bar{X}c^4}{24} + \frac{v}{720} = \frac{c^6}{720}, \quad \frac{Xc^6}{720} + \frac{\bar{X}c^5}{120} + \frac{v}{5040} = \frac{c^7}{5040}, \\ \frac{Xc^7}{5040} + \frac{\bar{X}c^6}{720} + \frac{v}{40320} = \frac{c^8}{40320}, \quad \frac{Xc^8}{40320} + \frac{\bar{X}c^7}{5040} + \frac{v}{362880} = \frac{c^9}{362880}, \end{gathered} \tag{29}$$

and the output order conditions are given as

$$\begin{gathered} b^T e = 1, \quad b^T c + \bar{b}^T e = \frac{1}{2}, \quad \frac{1}{2} b^T c^2 + \bar{b}^T c = \frac{1}{6}, \quad \frac{1}{6} b^T c^3 + \frac{1}{2} \bar{b}^T c^2 = \frac{1}{24}, \\ \frac{1}{24} b^T c^4 + \frac{1}{6} \bar{b}^T c^3 = \frac{1}{120}, \quad \frac{1}{120} b^T c^5 + \frac{1}{24} \bar{b}^T c^4 = \frac{1}{720}, \quad \frac{1}{720} b^T c^6 + \frac{1}{120} \bar{b}^T c^5 = \frac{1}{5040}, \\ \frac{bc^7}{5040} + \frac{\bar{b}c^6}{720} = \frac{1}{40320}, \quad \frac{bc^8}{40320} + \frac{\bar{b}c^7}{5040} = \frac{1}{362880}. \end{gathered} \tag{30}$$

Solving the order conditions (27) and (28), then setting $c = (0, 1, \frac{1}{3}, \frac{2}{3}, \frac{3}{4})^T$.

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b^T & \bar{b}^T \end{array} =$$

$$\begin{array}{c|c|ccccc|ccccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & \frac{313}{729} & \frac{-38}{729} & \frac{49}{729} & 0 & \frac{-1}{9} & 0 & \frac{4}{2187} & \frac{5}{2187} & \frac{-21}{81} & \frac{-21}{81} & 0 \\ \frac{2}{3} & \frac{416}{729} & \frac{-49}{729} & \frac{38}{729} & \frac{1}{9} & 0 & 0 & \frac{5}{2187} & \frac{4}{2187} & \frac{-21}{81} & \frac{-21}{81} & 0 \\ \frac{3}{4} & \frac{77409}{131} & \frac{-288063}{4194304} & \frac{208749}{4194304} & \frac{448335}{4194304} & \frac{299619}{4194304} & 0 & \frac{9693}{4194304} & \frac{7335}{4194304} & \frac{-48843}{4194304} & \frac{-88209}{4194304} & 0 \\ \hline & & 0 & \frac{35671}{287280} & \frac{5184}{16625} & \frac{55323}{10640} & \frac{-2080768}{448875} & \frac{1}{380} & \frac{61}{13680} & \frac{-297}{13300} & \frac{351}{2128} & \frac{512}{1995} \end{array} . \tag{31}$$

The stability function of the SDMIRK method (29) is

$$R(z) = \frac{1787114240 + 11378465280z + 3225594960z^2 + 54585900z^3 + 64691460z^4 + 4888512z^5 + 274095z^6 + 10441z^7 + 225z^8}{17871114240 + 6492648960z + 1423623600z^2 - 30977640z^3 + 39494220z^4 - 3704160z^5 + 344949z^6 - 20427z^7 + 675z^8},$$

whose boundary locus plot shown in Figure 3 suggests that the SDMIRK method (29) is $A(\alpha)-$stable.

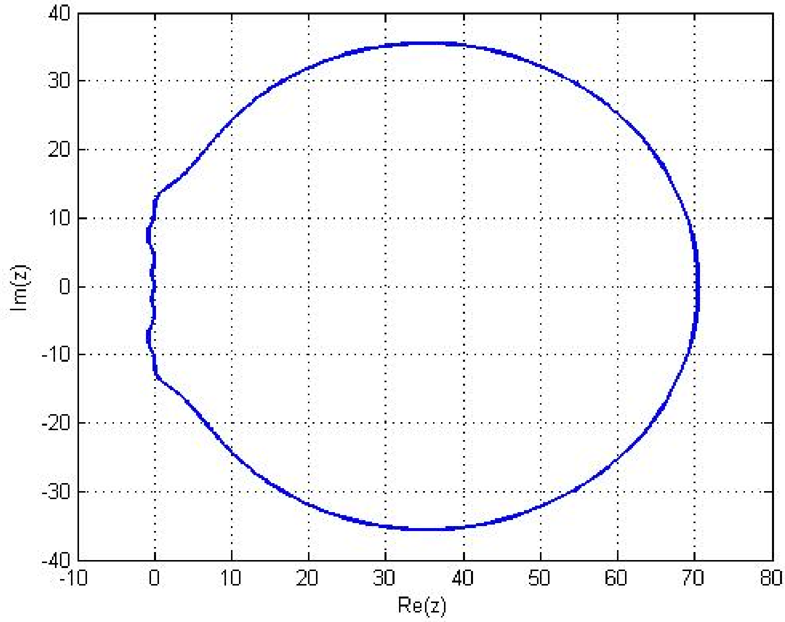

Figure 3: Boundary locus plot of the SDMIRK method (29).

4.4 Method of order $p = q = 11$; $s = 6$

The stage order conditions for the SDMIRK method (6) with $s = 6$ and of order $p = q = 11$ are given as

$$
\begin{gathered}
Xe + v = c, \quad Xc + \bar{X}e + \frac{v}{2} = \frac{c^2}{2}, \quad \frac{Xc^2}{2} + \bar{X}c + \frac{v}{6} = \frac{c^3}{6}, \quad \frac{Xc^3}{6} + \frac{\bar{X}c^2}{2} + \frac{v}{24} = \frac{c^4}{24}, \\
\frac{Xc^4}{24} + \frac{\bar{X}c^3}{6} + \frac{v}{120} = \frac{c^5}{120}, \quad \frac{Xc^5}{120} + \frac{\bar{X}c^4}{24} + \frac{v}{720} = \frac{c^6}{720}, \quad \frac{Xc^6}{720} + \frac{\bar{X}c^5}{120} + \frac{v}{5040} = \frac{c^7}{5040}, \\
\frac{Xc^7}{5040} + \frac{\bar{X}c^6}{720} + \frac{v}{40320} = \frac{c^8}{40320}, \quad \frac{Xc^8}{40320} + \frac{\bar{X}c^7}{5040} + \frac{v}{362880} = \frac{c^9}{362880} \\
\frac{Xc^9}{362880} + \frac{\bar{X}c^8}{40320} + \frac{v}{3628800} = \frac{c^{10}}{3628800}, \quad \frac{Xc^{10}}{3628800} + \frac{\bar{X}c^9}{362880} + \frac{v}{39916800} = \frac{c^{11}}{39916800},
\end{gathered}
\tag{32}
$$

and the output method order conditions are

$$
\begin{gathered}
b^T e = 1, \quad b^T c + \bar{b}^T e = \frac{1}{2}, \quad \frac{1}{2}b^T c^2 + \bar{b}^T c = \frac{1}{6}, \quad \frac{1}{6}b^T c^3 + \frac{1}{2}\bar{b}^T c^2 = \frac{1}{24}, \\
\frac{1}{24}b^T c^4 + \frac{1}{6}\bar{b}^T c^3 = \frac{1}{120}, \quad \frac{1}{120}b^T c^5 + \frac{1}{24}\bar{b}^T c^4 = \frac{1}{720}, \quad \frac{1}{720}b^T c^6 + \frac{1}{120}\bar{b}^T c^5 = \frac{1}{5040}, \\
\frac{bc^7}{5040} + \frac{\bar{b}c^6}{720} = \frac{1}{40320}, \quad \frac{bc^8}{40320} + \frac{\bar{b}c^7}{5040} = \frac{1}{362880} \\
\frac{bc^9}{362880} + \frac{\bar{b}c^8}{40320} = \frac{1}{3628800}, \quad \frac{bc^{10}}{3628800} + \frac{\bar{b}c^9}{362880} = \frac{1}{39916800}.
\end{gathered}
\tag{33}
$$

Solving the system of equations (30) and (31), then setting $c = (0, 1, \frac{1}{2}, \frac{2}{3}, \frac{3}{4}, \frac{4}{3})^T$, we have the SDMIRK method

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b^T & \bar{b}^T \end{array} \tag{34}$$

where

$$v = \left(0, 0, \frac{184991}{2023391}, \frac{195808}{203391}, \frac{3912057}{40636232}, \frac{32783360}{203391}\right)^T,$$

$$X = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{-220042}{3050865} & \frac{757079}{82373355} & \frac{-64412}{523125} & \frac{-3421}{4185} & \frac{4399824896}{10296669375} & 0 \\ \frac{-223757}{3050865} & \frac{323974}{82373355} & \frac{-1567}{523125} & \frac{-6236}{4185} & \frac{13040091136}{10296669375} & 0 \\ \frac{-47675871}{650117120} & \frac{2551701}{650117120} & \frac{-242159949}{81264640000} & \frac{-940827717}{650117120} & \frac{50637}{38750} & 0 \\ \frac{-16782496}{3050865} & \frac{-1416929788}{82373355} & \frac{-73376}{523125} & \frac{-12685472}{4185} & \frac{-32113470472192}{10296669375} & 0 \end{bmatrix},$$

$$\bar{X} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{4136}{3250865} & \frac{1439}{5491557} & \frac{-3314}{313875} & \frac{-79}{12555} & \frac{-31981568}{686444625} & 0 \\ \frac{4811}{3050865} & \frac{640}{5491557} & \frac{-799}{313875} & \frac{-794}{12555} & \frac{-52953088}{686444625} & 0 \\ \frac{1024893}{650117120} & \frac{15123}{130023424} & \frac{-41275251}{16252928000} & \frac{40684761}{650117120} & \frac{-9633}{124000} & 0 \\ \frac{8752288}{3050865} & \frac{-2856805}{5491557} & \frac{3048928}{313875} & \frac{1908848}{12555} & \frac{88852135936}{686444625} & 0 \end{bmatrix},$$

$$b^T = \begin{bmatrix} 0 & \frac{1172327}{10644480} & \frac{8328}{89375} & \frac{-493371}{80080} & \frac{40336031744}{57593913125} & \frac{7265463}{1757916160} \end{bmatrix},$$

and

$$\bar{b}^T = \begin{bmatrix} 70380080 & \frac{79081}{23063040} & \frac{-102561}{2002000} & \frac{-267651}{640640} & \frac{-1122304}{6131125} & \frac{35313}{125565440} \end{bmatrix}.$$

The stability function of the SDMIRK method (32) is

$$R(z) = \frac{P(z)}{Q(z)},$$

where

$$P(z) = A(z) + B(z),$$
$$Q(z) = C(z) + D(z),$$

and

$$A(z) = -281448886118400 - 314202405888000z - 95083542550080z^2 \\ -14280918321600z^3 - 1212571571400z^4,$$

$$B(z) = -51385155840z^5 + 573366600z^6 + 231709440z^7 + 16163478z^8 \\ +614829z^9 + 11771z^{10},$$

$$C(z) = -281448886118400 - 32753519769600 + 78394420278720z^2 \\ -29390431029120z^3 + 6166606201560z^4,$$

$$D(z) = -878375181240z^5 + 91463669100z^6 - 7163579436z^7 + 420059499z^8 \\ -17487342z^9 + 423756z^{10}.$$

whose boundary locus plot (shown in Figure 4) shows that it is $A(\alpha)-$stable.

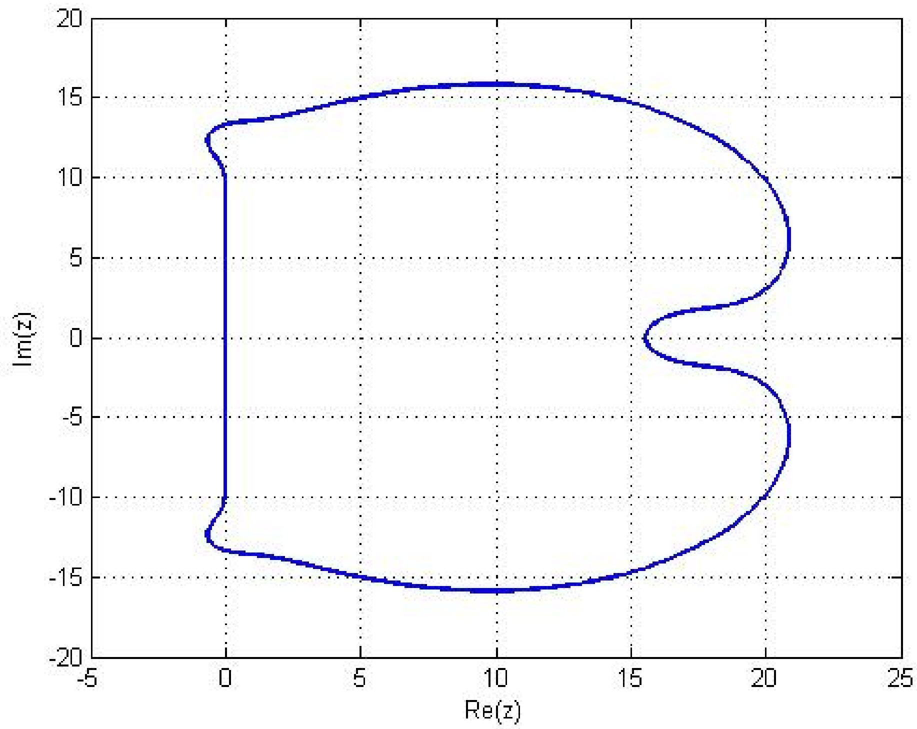

Figure 4: Boundary locus plot of the SDMIRK method (32).

5 Numerical Experiment

The implementation of the SDMIRK method (6) is discussed herein. A test example is carried out by implementing the sixth order SDMIRK method (23) on some stiff problems and the results of the sixth order SDMIRK method (23) are compared with the results of some existing methods (which includes, the six order second derivative linear multi-step method (SDLMM) of [23] and the sixth order second derivative backward difference formula (SDBDF) [20]).

Since the stages of the SDMIRK method (6) are implicit, we resolve its implicitness using the Newton's method. To carry out this, the non-linear equation defining the implicit stage values are

$$Y_r = (1 - v_r)y_n^{[j]} + v_r y_{n+1}^{[j]} + h \sum_{i=1}^{r-1} x_{ri} f(y_r^{[j]}) + h^2 \sum_{i=1}^{s} \bar{x}_{ri} g(y_r^{[j]}). \tag{35}$$

Thus, resolving the implicitness by the Newton's method gives,

$$Y_r^{[j+1]} = Y_r^{[j]} - \left(I_s - hXJ(Y_r^{[j]}) - h^2 \bar{X} J'(Y_r^{[j]})\right)^{-1} F(Y_r^{[j]}), \tag{36}$$

where J and J' are the Jacobian matrices,

$$J(Y_r^{[j]}) = \frac{\partial f_i}{\partial y_j}; \qquad J'(Y_r^{[j]}) \approx \left(\frac{\partial f_i}{\partial y_j}\right)^2. \tag{37}$$

Our starting values for the SDMIRK method (23) is obtained from the explicit Euler scheme

$$y_{n+1} = y_n + hf_n. \tag{38}$$

We implement the SDMIRK method (23), SDLMM [23] and SDBDF [20] of the following non-linear stiff problems.

Problem 1 [18]

$$\begin{aligned} &y_1' = -8y_1 + 7y_2, \quad y_1(0) = 1, \quad y_1(x) = 2e^{-x} - e^{-50x}, \\ &y_2' = 42y_1 - 43y_2, \quad y_2(0) = 8, \quad y_2(x) = 2e^{-x} + 6e^{-50x}, \\ &\quad x \in [0, 15]. \end{aligned} \tag{39}$$

Problem 2 [1]

$$\begin{aligned} &y_1' = -10004y_1 + y_2^4, \quad y_1(0) = 1, \quad y_1(x) = e^{-4x}, \\ &y_2' = y_1 - y_2(1 + y_2^3), \quad y_2(0) = 1 \quad y_2(x) = e^{-x}, \\ &\quad x \in [0, 15]. \end{aligned} \tag{40}$$

Problem 3 [27]

$$y'(x) = 10^4 \left(y - \phi(x) + \phi'(x)\right), \quad y(0) = \phi(0), \quad y(x) = \phi(x)$$
$$\phi(x) = sinx, \tag{41}$$

Tables 5.1–5.3 shows the results of the SDMIRK method (23), SDLMM [23] and SDBDF [20] when implemented on problems 1–3. In the tables, the absolute global error are presented.

Table 5.1 shows that the error obtained from the SDMIRK method (23) is far smaller than that obtained from the SDLMM [23] and SDBDF [20] methods. Hence SDMIRK method (23) gives better accuracy. The results in Table 5.2 confirms that the SDMIRK method (23) performs better than SDLMM [23] and SDBDF [20]. Again, Table 5.3 shows that the error from the SDMIRK method (23) is better than that of the SDLMM [23] and SDBDF [20].

Table 5.1: Numerical results of problem 1 for $h = 10^{-2}$.

x	y_n	Error in SDMIRK (23)	Error in SDLMM [23]	Error in SDBDF [20]
5.0	y_1	5.5196×10^{-13}	2.8297×10^{-6}	4.4683×10^{-6}
	y_2	5.5196×10^{-13}	2.8297×10^{-6}	4.4683×10^{-6}
10.0	y_1	7.4412×10^{-15}	1.9066×10^{-8}	3.0107×10^{-8}
	y_2	7.4412×10^{-15}	1.9066×10^{-8}	3.0107×10^{-8}
15.0	y_1	7.5199×10^{-17}	1.2847×10^{-10}	2.0286×10^{-10}
	y_2	7.5199×10^{-17}	1.2847×10^{-10}	2.0286×10^{-10}

Table 5.2: Numerical results of problem 2 for $h = 10^{-2}$.

x	y_n	Error in SDMIRK (23)	Error in SDLMM [23]	Error in SDBDF [20]
5.0	y_1	7.4988×10^{-15}	1.731×10^{-12}	2.0611×10^{-9}
	y_2	4.373×10^{-9}	6.7380×10^{-3}	6.7379×10^{-3}
10.0	y_1	1.5456×10^{-23}	4.5400×10^{-5}	2.1730×10^{-3}
	y_2	2.9468×10^{-11}	4.5400×10^{-2}	4.5399×10^{-5}
15.0	y_1	3.1857×10^{-32}	3.0590×10^{-23}	2.0286×10^{-23}
	y_2	1.9855×10^{-13}	2.0230×10^{-7}	3.0450×10^{-7}

Table 5.3: Numerical results of problem 3 for $h = 10^{-2}$.

x	y_n	Error in SDMIRK (23)	Error in SDLMM [23]	Error in SDBDF [20]
0.2	y	4.2353×10^{-7}	5.7636×10^{-3}	1.8865×10^{-1}
0.4	y	3.8585×10^{-7}	0.11495×10^{-1}	3.7939×10^{-1}
0.6	y	3.3278×10^{-7}	1.6756×10^{-2}	5.5462×10^{-1}
0.8	y	2.6645×10^{-7}	2.133×10^{-2}	7.0733×10^{-1}
1.0	y	1.8949×10^{-7}	2.5056×10^{-2}	8.3144×10^{-1}

6 Conclusion

In this paper, a class of generalised SDMIRK methods have been introduced. This method is an extension of MIRK method discussed in [18]. The SDMIRK method (6) derived in section (4) reveals that the new schemes enjoyed A-stability and $A(\alpha)$-stability properties. The SDMIRK methods (23), SDLMM [23] and SDBDF [20] have been implemented on problems 1–3 and the results obtained show that the SDMIRK outperforms SDLMM [23] and SDBDF [20].

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