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EXTENDED MONO-IMPLICIT RUNGE-KUTTA METHODS FOR STIFF ODES

I.B. Aihie and R.I. Okuonghae

Department of Mathematics, University of Benin, Benin City; Nigeria.

Abstract:

An extended Mono Implicit Runge-kutta (EMIRK) method is considered herein for the numerical solution of stiff initial value problems (IVPs) in ordinary differential equation (ODEs). The methods are A-stable for $p = 6, 8$ and 10 . The p and q are the order of the input and output methods respectively. Numerical results are given to illustrate the application of the new methods.

Keywords: Second derivative Mono-Implicit Runge-Kutta method; order condition; stiff IVPs; A-stability.

1. Introduction

The Mono- Implicit Runge-Kutta (MIRK) method first presented in [1], is a sub-class of the Implicit Runge-Kutta (IRK) method presented in [2] for the numerical solution of stiff ODEs. The method in [1] emerged in order to circumvent the computational cost involve in IRK method. Over the years considerable attention has been devoted to the MIRK methods because of its efficiency in implementation compare to other subclasses of the IRK methods studied [3, 4]. In 1993, Muir and Owren [5] studied the continuous version of the Mono-implicit Runge-Kutta Schemes which uses a minimal number of stages for order 1 to 6. Burrage et al [6] in their paper give a complete characterization of some subclasses of these methods having a number of stages $s \leq 5$ and also proof that the order of an s-stage MIRK method is at most $s + 1$. De Meyer et al [7], studied the condition to be met by Mono-implicit Runge-Kutta method in order to generate a Mono-implicit Runge-Kutta-Nystrom (MIRKN) method that are $p - stable$. Muir and Adams [8] studied Mono-implicit Runge-Kutta-Nystrom (MIRKN) methods that are suitable for system of second order ODEs and derived optimal symmetric methods of order 2, 4 and 6 .The MIRK method suffer from order reduction when applied to certain stiff ODEs, in order to address these problem, Dow [9], developed a family of generalized MIRK methods that do not suffer order reduction when applied to stiff ODEs. The methods proposed by Dow [9] do not have second derivative terms, therefore, the need to search for methods with high order, accuracy and stability good properties and also retained computational advantage of the MIRK methods leads to the extended mono-implicit Runge-Kutta (EMIRK) method. The idea of the second derivative terms was first introduced by Enright [10] for stiff ODEs. The use of second derivative terms in explicit methods has been proposed for non-stiff problems by many authors for example see Chan and Tsai [11], Okuonghae [12], Turaci and Ozis [13], Aiguobasimwin and Okuonghae [54]. Similarly, for stiff ODEs some authors have proposed implicit methods that incorporate the second derivative terms in their methods see Butcher and Hojjati [11], Abdi and Hojjati [16,17], Okuonghae and Ikhile [18] ,Okuonghae and Ikhile in [19] , Ogunfeyitimi and Ikhile [20] **,** Nwachukwu and Okor [21]. In the spirit of the authors in the literature, we introduce a class of second derivative mono implicit methods for stiff ODEs.

2. Formulation of the method for ODEs

For the initial value problems (IVP)

$$y' = f(x,y), \quad y'' = f_x + f_y f = g(x,y), \quad x\epsilon[x_0, X] \quad y(x_0) = y_0 \qquad (1)$$

where $f\colon \mathbb{R}^s \to \mathbb{R}^s$ and $g\colon \mathbb{R}^s \to \mathbb{R}^s$. We define the EMIRK method as

$$Y_r = (1 - v_r)y_n + v_r y_{n+1} + h\sum_{j=1}^{r-1} x_{rj} f(x_n + c_j h, Y_j) + h^2 \sum_{j=1}^{r-1} \bar{x}_{rj} g(x_n + c_j h, Y_j), c_r\epsilon(0,1), \quad r - 1,2 \dots s \qquad (2)$$

and

$$y_{n+1} = y_n + h\sum_{r=1}^{s} b_r(1) f(x_n + c_r h, Y_r) + h^2 \sum_{r=1}^{s} \bar{b}_r(1) g(x_n + c_r h, Y_r), \ \theta = 1 \qquad (3)$$

The $g(x,y)$ is the second derivative form of ODEs in (1), $c_r = (c_1, \ \ . . ., c_s)^T$ is the abscissa value and $Y_r = y(x_n + c_r h)$, the coefficients, $\{v_r\}_{r=1}^{s}$, $\{x_{rj}\}_{j=1,r=1}^{r-1,s}$, $\{\bar{x}_{rj}\}_{j=1,r=1}^{r-1,s}$, defined the stages, $\{b_r(\theta)\}_{r=1}^{s}$ and $\{\bar{b}_r(\theta)\}_{r=1}^{s}$ are the weight polynomials. We shall require $c_r = \sum_{j=1}^{r-1} x_{rj} + \sum_{j=1}^{r-1} \bar{x}_{rj} + v_r$ and $\theta = 1$ i.e $b_r(1) = b_r$ and $\bar{b}_r(1) = \bar{b}_r$. Equation (2) is an extension of the methods in [15], and a subclass of the methods in [2, 22]. A survey of some second derivative A-stable methods can be found in [[15], [21], [19],]. The paper is organized as follows. In section 2, the order condition and stability analysis of the EMIRK methods are stated. Section 3 is devoted to the derivation of the EMIRK methods and section 4, numerical results are presented.

Corresponding Author**:** Aihie I.B., Email: becsin2002@yahoo.co.uk, Tel: +2348098107785

The Butcher tableaux of the methods in (2) is

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b(1)^T & \bar{b}(1)^T \end{array} = \begin{array}{c|c|c|c} c_1 & v_1 & X_{11} \ldots\ldots\ X_{1s} & \bar{X}_{11}\ \ldots\ldots\ \bar{X}_{1s} \\ \vdots & \vdots & \vdots & \vdots \\ c_s & v_1 & X_{1s} \ldots\ldots\ X_{ss} & \bar{X}_{11}\ \ldots\ldots\ \bar{X}_{1s} \\ \hline & & b_1(1)^T\ \ldots\ b_s(1)^T & \bar{b}_1(1)^T\ \ldots\ \bar{b}_s(1)^T \end{array} \qquad (4)$$

Where$c = (c_1, \ . \ . \ ., c_s)^T$,$v = (v_1, \ . \ . \ ., v_s)^T$,$b = (b_1(1), \ . \ . \ ., b(1)_s)^T$, $\bar{b} = (\bar{b}_1(1), \ . \ . \ ., \bar{b}_s(1))^T$, $X \ and \ \bar{X}$ are the s by s matrix whose $(i\ , j)th$ component are x_{ij} and $\bar{x}_{ij}$.

3. The order condition of the EMIRK methods

The order conditions of the methods in (2) are obtained by Taylor's series expansion approach about x_n and equating the power of h to zero gives stage order q

$C = Xe + v$;

$$\frac{c^j}{j!} = \frac{Xc^{j-1}}{(j-1)!} + \frac{\bar{X}c^{j-2}}{(j-2)!} + \frac{v}{j!} \quad j = 2(1)q, \qquad (5)$$

and the method of order p

$$b^T e = e \qquad (6)$$

$$\frac{1}{j!} = \frac{b^T c^{j-1}}{(j-1)!} + \frac{\bar{b}^T c^{j-2}}{(j-2)!} + \frac{v}{j!} \quad j = 2(1)\ p.$$

4. Stability Analysis

In this section our interest is on the analysis of the stability of the method in (2) in what follows is the derivation of the stability function of the method in (2).

Theorem 4.1: let $R(z)$ denote the stability function for an EMIRK method. Then for a linear differential equation $y(x)' = \lambda y(x)$, the methods in (2) and (3) has the stability function

$$R(z) = \frac{I - zX - z^2\bar{X} + zeb^T + z^2\bar{b}^T - zvb^T - z^2 v\bar{b}^T}{I - zX - z^2\bar{X} - zvb^T - z^2 v\bar{b}^T}, \ z = \lambda h. \qquad (7)$$

Proof: for the special problem defined by $y' = \lambda y(x)$, the stages derivatives f and $y'' = g$ is related to the stage values Y by $f = \lambda y$ and $g = \lambda^2 y$. To ease our prove, we take $e = (1, \ldots, 1)^T$ and $v = (v_1 \ldots, v_s)^T$, Hence, (2) reduces to the form

$$(I - zX - z^2\bar{X})Y - vy_{n+1} = (e - v)y_n \qquad (8)$$

and

$$\left(-zb^T - z^2\bar{b}^T\right)Y + y_{n+1} = y_n \qquad (9)$$

From (8) we have,

$$Y = \frac{(e-v)y_n + vy_{n+1}}{(I - zX - z^2\bar{X})} \qquad (10)$$

Inserting (10) into (9) gives

$$\left(-zb^T - z^2\bar{b}^T\right)\left(\frac{(e-v)y_n + vy_{n+1}}{(I - zX - z^2\bar{X})}\right) + y_{n+1} = y_n \qquad (11)$$

Multiplying both side of the (11) by $(I - zX - z^2\bar{X})$ gives

$$\left(-zb^T - z^2\bar{b}^T\right)\left((e-v)y_n + vy_{n+1}\right) + (I - zX - z^2\bar{X})y_{n+1} = (I - zX - z^2\bar{X})y_n \qquad (12)$$

Simplifying (12) and collecting like terms yields

$$\left[v\left(-zb^T - z^2\bar{b}^T\right) + (I - zX - z^2\bar{X})\right]y_{n+1} = \left[(I - zX - z^2\bar{X})(e - v)\left(-zb^T - z^2\bar{b}^T\right)\right]y_n. \quad (13)$$

From (13) we obtain $y_{n+1} = R(z)y_n$. Thus the stability function is

$$R(z) = \frac{I - zX - z^2\bar{X} + zeb^T + z^2\bar{b}^T - zvb^T - z^2 v\bar{b}^T}{I - zX - z^2\bar{X} - zvb^T - z^2 v\bar{b}^T} \qquad (14)$$

5. Construction of the EMIRK methods

In this section, we will derive method (2) that has order p not equal to stage order q. The approach adopted here, in the derivation of the method in (2) is similar to that used in [19] and [23].

5.1 **EMIRK method of order** p=1, **s**=1

For example, fixing $r = 1$, and $v_1 = 0$ in (2) gives

$$Y_1 = y_n \qquad (15)$$

Similarly, we obtain the output method of order $p = 1$ in (3). That is

$$y_{n+1} = y_n + hf(x_n, Y_1) \qquad (16)$$

The tableau for (15) is

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b(1)^T & \bar{b}(1)^T \end{array} \quad = \quad \begin{array}{c|c|c|c} 0 & 0 & 0 & 0 \\ \hline & & 1 & 0 \end{array} \qquad (17)$$

The method in (15 and 16) in an explicit Euler's method, which is not of interest in this paper but such scheme are suitable for non-stiff ODEs. The Euler's scheme has an interval of absolute stability of [-2, 0].

5.2 **EMIRK method of order** *p*=3, **s**=2

Take $r = 2$ in (2) and fix $v_1 = 1$ gives

$$Y_1 = y_n$$
$$Y_2 = y_{n+1} \qquad (18)$$
$$y_{n+1} = y_n + \frac{2h}{3} f(x_n, Y_1) + \frac{h}{3} f(x_{n+1}, Y_2) + \frac{h^2}{6} g(x_n, Y_1)$$

The picture of the scheme in (18) is

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b(1)^T & \bar{b}(1)^T \end{array} \quad = \quad \begin{array}{c|c|cc|cc} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ \hline & & \frac{2}{3} & \frac{1}{3} & \frac{1}{6} & 0 \end{array} \qquad (19)$$

The algorithm in (18) is of order *p*=3, the interval of absolute stability of the method is [-2, 0] and such scheme is good for the numerical solution of non-stiff ODEs (1). Our interest in this study is implicit Runge-Kutta method. Therefore, we give below some suitable methods emanating from (2) and (3) for stiff problems (1).

5.3 **EMIRK method of order** *p*=6, *q*=5, **s**=3

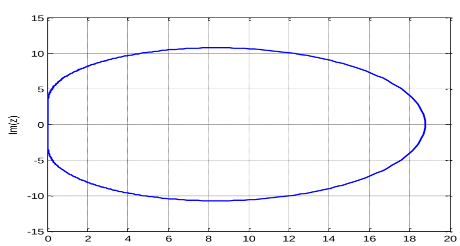
Fixing p=6, *q*=5, s=3 in (5) and (6) and solving the resulting system of linear equations in terms of $\{c_r\}_{r=1}^{3}$ such that $c_1 \neq c_2 \neq c_3$. The resulting tableau of the method of order *p*=6 is

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b(1)^T & \bar{b}(1)^T \end{array} \quad = \quad \begin{array}{c|c|ccc|ccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{4} & \frac{1836}{2048} & \frac{78}{2048} & \frac{-378}{2048} & 0 & \frac{9}{2048} & \frac{27}{2048} & 0 \\ \hline & & \frac{458}{1620} & \frac{1674}{1620} & \frac{-512}{1620} & \frac{39}{1620} & \frac{-135}{1620} & \frac{-384}{1620} \end{array} \qquad (20)$$

The stability function of the method in (20) is $R(z) = -\frac{-960-204z+12z^2+10z^3+z^4}{960-720z+228z^2-38z^3+3z^3}$ and plotting the stability function of (20) in boundaries locus sense shows that the scheme in (20) is $A - stable$.

Note: In the other part of this paper, the EMIRK method of order *p*=6, *q*=5, s=3 is represented by EMIRK6.

Figure 1: Stability plot for EMIRK6



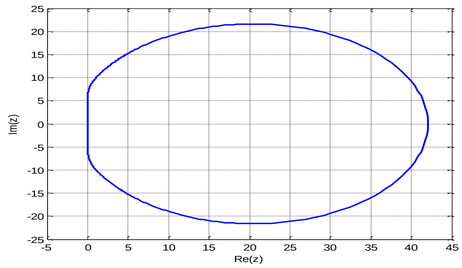
5.4 **EMIRK method of order** *p*=8, *q*=7, **s**=4

Similarly, setting p=8, *q*=7, s=4 in (5) and (6) and solving the resulting system of linear equations in terms of $\{c_r\}_{r=1}^{4}$ such that $c_1 \neq c_2 \neq c_3 \neq c_4$.The resulting tableau of the method of order p=8 is;

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b(1)^T & \bar{b}(1)^T \end{array} = \begin{array}{c|c|cccc|cccc} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{96}{192} & \frac{18}{192} & \frac{-18}{192} & 0 & 0 & \frac{1}{192} & \frac{1}{192} & \frac{-8}{192} & 0 \\ \frac{3}{4} & \frac{5724}{8192} & \frac{474}{8192} & \frac{-918}{8192} & \frac{864}{8192} & 0 & \frac{27}{8192} & \frac{45}{8192} & \frac{-144}{8192} & 0 \\ \hline & & \frac{1910}{11340} & \frac{3510}{11340} & \frac{-4320}{11340} & \frac{10240}{11340} & \frac{93}{11340} & \frac{-189}{11340} & \frac{-1728}{11340} & \frac{-1536}{11340} \end{array} \quad (21)$$

The stability function of the method in (21) is $R(z) = -\frac{-161280-40320z+480z^2+1440z^3+252z^4+22z^5+z^6}{161280-120960z+39840z^2-7680z^3+948z^4-74z^5+3z^6}$ and the method in (21) is $A-stable$ has showed in the stability plot in Figure 2.

Figure 2: Stability plot for EMIRK8



5.5 **EMIRK method of order** *p*=10, *q*=9, **s**=5

Setting s=5, $c = (0,1,\frac{1}{3},\frac{2}{3},\frac{4}{5})^T$ in (5) and (6) yield the EMIRK methods of order 9 with the modified Butcher tableaux of the resulting coefficients given below.

$$\begin{array}{c|c|c|c} c & v & X & \bar{X} \\ \hline & & b(1)^T & \bar{b}(1)^T \end{array} \qquad v = (0,1,\frac{939}{2187},\frac{1248}{2187},\frac{1269760}{1953125})^T \qquad (22)$$

$$X = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \frac{147}{2187} & \frac{-114}{2187} & 0 & \frac{-243}{2187} & 0 \\ \frac{114}{2187} & \frac{-147}{2187} & \frac{243}{2187} & 0 & 0 \\ \frac{83300}{1953125} & \frac{-140480}{1953125} & \frac{181440}{1953125} & \frac{168480}{1953125} & 0 \end{bmatrix}$$

$$\bar{X} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \frac{5}{2187} & \frac{4}{2187} & \frac{-54}{2187} & \frac{-27}{2187} & 0 \\ \frac{4}{2187} & \frac{5}{2187} & \frac{-27}{2187} & \frac{-54}{2187} & 0 \\ \frac{2936}{1953125} & \frac{4544}{1953125} & \frac{-19008}{1953125} & \frac{-30672}{1953125} & 0 \end{bmatrix}$$

$$b^T = \begin{bmatrix} \frac{2076865}{18439680} & \frac{4253200}{18439680} & \frac{2507760}{18439680} & \frac{-40007520}{18439680} & \frac{49609375}{18439680} \end{bmatrix}$$

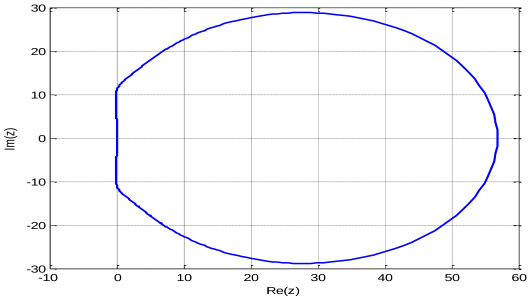
$$\bar{b}^T = \begin{bmatrix} \frac{66542}{18439680} & \frac{-159152}{18439680} & \frac{-843696}{18439680} & \frac{-4667544}{18439680} & \frac{-3281250}{18439680} \end{bmatrix}$$

The stability function is

$$R(z) = -\frac{-183708000 - 36741600z + 4173120z^2 + 2426760z^3 + 417390z^4 + 41790z^5 + 2742z^6 + 119z^7 + 3z^8}{183708000 - 146966400z + 50939280z^2 - 10500840z^3 + 1453710z^4 - 142260z^5 + 9903z^6 - 466z^7 + 12z^8}.$$

The stability plot for the method of order $p = 10$ in Figure 3 shows that the method in (22) is $A - stable$

Figure 3: Stability plot for EMIRK10



6. Numerical Experiment

In this section, we present numerical results showing the implementation and accuracy of the constructed EMIRK6,

$$\begin{array}{c|c|ccc|ccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{3}{4} & \frac{1836}{2048} & \frac{78}{2048} & \frac{-378}{2048} & 0 & \frac{9}{2048} & \frac{27}{2048} & 0 \\
\hline
 & & \frac{190}{540} & \frac{-162}{540} & \frac{512}{540} & \frac{21}{540} & \frac{27}{540} & 0
\end{array}$$

Our interest here is to compare the results of our methods with the results obtained from some existing methods of order 6. The Maximum Error= $Max\|y_i - y(x_i)\|$ represents error between the computed solution $y(x_i)$ and the exact solution y_i. The order of EMIRK6 is $p = 6$, see section 5 of this article. Computational experiments are done by applying the EMIRK6 methods to the following problems:

Problem 1: Consider the system of differential equations [20],

$$\begin{cases} y_1'(x) = -21y_1 + 19y_2 - 20y_3, & y_1(x) = \frac{1}{2}\left(e^{-2x} + e^{-40x}(\cos(40x) + \sin(40x))\right), \\ y_2'(x) = 19y_1 - 21y_2 + 20y_3, & y_2(x) = \frac{1}{2}\left(e^{-2x} - e^{-40x}(\cos(40x) - \sin(40x))\right), \\ y_3'(x) = 40y_1 - 40y_2 - 40y_3, & y_2(x) = -e^{-40x}(\cos(40x) - \sin(40x)), \\ x\epsilon[0,1], & y(0) = [1, 0, -1]^T \end{cases}$$

We have solved this problem at $h = 0.05, 0.025, 0.0125$ and 0.00625 and compared the result with method GSDLMM [20] and BVMs [24].

Table 1: Numerical results for problem 1 on interval $0 < x \leq 1$.

x	EMIRK6 (20) (rate)	GSDLMM ($p = 6$)[20] (rate)	BVMs($p = 6$)[24] (rate)
0.05	2.67×10^{-3} (--)	3.0×10^{-2} (--)	5.70×10^{-2} (--)
0.025	8.92×10^{-5} (4.9)	3.55×10^{-3} (3.07)	8.70×10^{-3} (2.70)
0.0125	$1.37.0 \times 10^{-6}$ (6.02)	2.226×10^{-4} (3.97)	4.90×10^{4} (4.20)
0.00625	1.92×10^{-8} (6.15)	5.86×10^{-6} (5.27)	1.20×10^{-5} (5.40)

Table 1 show that the new method EMIRK6 performs better in terms of accuracy than the existing method herein and are well suited for the integration of stiff system in ODEs.

Problem 2: Non-linear stiff system [20],

$$\begin{cases} y_1' = -1002y_1 + 1000y_2^2, & y_1(x) = e^{-2x}, \\ y_2' = y_1 - y_2(1 + y_2), & y_2(x) = e^{-x} \\ x \in [0,1], \quad y(0) = [1,1]^T \end{cases}$$

Table 2: the results of the numerical integration at $N = 125$ are presented to show the results for the EMIRK6 (20), SDAM [25] and BVMs [24] on problem 2 for fixed step size $h = 0.008$.

Method	Order	N	h	y_1 (Max$\|y_i - y(x_i)\|$)	y_2 (Max$\|y_i - y(x_i)\|$)
EMIRK6(20)	6	125	0.008	6.200×10^{-17}	5.55×10^{-17}
SDAM [25]	6	125	0.008	1.63×10^{-14}	0.00
BVMs [24]	6	125	0.008	6.61×10^{-12}	6.74×10^{12}

In like manner, the numerical results in Table 2 show that the new methods are capable of giving accurate and stable results, hence EMIRK6 is better in terms of accuracy than the SDAM [25] and BVMs [24].

7. Conclusion

In this paper, a family of A-stable EMIRK method is proposed for the numerical solution of stiff IVPs in ODEs. The stability analysis in section 4 and the plot in Fig. 1-3 show that the methods possess zero and A-stability properties. The numerical results in Table 1-2 is an evident that the proposed methods perform better than some existing methods in the literature, see Table 1-2.

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