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THIRD DERIVATIVE MONO-IMPLICIT RUNGE-KUTTA METHODS FOR STIFF ODEs

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ABSTRACT

This work focuses on a Third-Derivative Mono-Implicit Runge–Kutta (TD-MIRK) method developed for the numerical approximation of stiff initial value problems (IVPs) in ordinary differential equations. The order conditions for the scheme are derived using Taylor series expansions. We introduce a seventh-order TD-MIRK method constructed to require the least possible number of function evaluations. The numerical experiments are then compared with well-known methods previously reported in the literature.

1. INTRODUCTION

The study, investigate a Third-Derivative Mono-Implicit Runge–Kutta (TD-MIRK) methods developed for the numerical solution of initial value problems (IVPs) associated with ordinary differential equations (ODEs):

$$y' = f(x, y), x \epsilon [x_0, X] \;\; y(x_0) = y_0$$

where $g = y'' = f_x + \; f_y f \;\; l = y''' = f_{xx} + \; 2ff_{xy} + f^2 f_{yy} + f_x f_y f + ff_{Yy}, \;\; f: \mathbb{R}^N \to \mathbb{R}^N$ and $l: \mathbb{R}^N \to \mathbb{R}^N$. Numerous real-world applications can be represented by (1). The MIRK method was first presented in [10] with its general form expressed as

$$Y_i = (1 - v_i)y_n + v_i y_{n+1} + h \sum_{j=1}^{i-1} x_{ij} f\left(x_n + c_j h, Y_j\right), i = 1,2, \dots s,$$

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i). \qquad (2)$$

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Here, $c = [c_1, \ldots, c_s]^T$, and h are the abscissa vector and step-size respectively. The $Y_i = y(x_n + c_i h)$ and y_{n+1} are approximation of the stage and output methods of order q and p Respectively. The corresponding tableau to the method in (2) is given as follows

c	v	X
		b^T

Several modifications of the MIRK methods has been proposed in [7],[11],[13],[14],[15] and[16]. Recently, Aihie and Okuonghae [2-4] enhanced the formulation of MIRK method frameworks through the inclusion of second derivative term, as presented in equation (3) below.

$$Y_i = (1 - v_i)y_n + v_i y_{n+1} + h\sum_{j=1}^{i-1} x_{ij} f(x_n + c_j h, Y_j) + h^2 \sum_{j=1}^{i-1} \bar{x}_{ij} g(x_n + c_j h, Y_j), \quad i = 1,2 \ldots s$$

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i f(x_n + c_i h, Y_i) + h^2 \sum_{i=1}^{s} \bar{b}_i g(x_n + c_i h, Y_i). \qquad (3)$$

Their approach was motivated by the need to improve accuracy and efficiency in solving a specific type of difficult differential equations (stiff ODEs). In the spirit of the authors in the literature, we incorporate the third derivative term in our method.

The TD-MIRK methods

An extended version of (3) consider in this paper is

$$Y_r = (1 - v_r)y_n + v_r y_{n+1} + h\sum_{j=1}^{r-1} x_{rj} f(x_n + c_j h, Y_j) + h^2 \sum_{j=1}^{r-1} \bar{x}_{rj} g(x_n + c_j h, Y_j) + h^3 \sum_{j=1}^{r-1} \hat{x}_{rj} g(x_n + c_j h, Y_j), c_r \in (0,1) \qquad (4)$$

And

$$y_{n+1} = y_n + h\sum_{r=1}^{s} b_i(\theta) f(x_n + c_r h, Y_r) + h^2 \sum_{r=1}^{s} \bar{b}_r(\theta) g(x_n + c_r h, Y_r) + h^3 \sum_{r=1}^{s} \hat{b}_r(\theta) g(x_n + c_r h, Y_r), \quad \theta = 1. \qquad (5)$$

The term l represents the third derivative in the system of ODEs given in (1), while $c_r = (c_1, \ldots, c_s)^T$, $Y_r = y(x_n + c_r h)$, $\{v_r\}_{r=1}^{s}, \{x_{rj}\}_{j=1,r=1}^{r-1,s}$, $\{\bar{x}_{rj}\}_{j=1,r=1}^{r-1,s}$, $\{\hat{x}_{rj}\}_{j=1,r=1}^{r-1,s}$, $\{b_r(\theta)\}_{r=1}^{s}$, $\{\bar{b}_r(\theta)\}_{r=1}^{s}$ and $\{\hat{b}_r(\theta)\}_{r=1}^{s}$ are defined as abscissa values, stages and the weight Polynomial. This method is derived under the condition that $c_r = \sum_{j=1}^{r-1} x_{rj} + \sum_{j=1}^{r-1} \bar{x}_{rj} + v_r$ and set $\theta = 1$. Equation (4) and (5) is an extension of the methods in [[2],[3], [4]]. Survey of some third derivative A-stable methods appear in [[6],[5],[18]]. Sections 3 and 4 cover order conditions and stability; Sections 5 and 6 derive the TD−MIRK schemes and the corresponding numerical experiments. The Butcher tableau associated with (4) and (5) is given by

c	v	X	$\bar{X}$	$\hat{X}$ =
		$b^T($	$\bar{b}^T$	$\hat{b}^T$

c_1	v_1	x_{11}	$\cdots$	x_{1s}	$\bar{\bar{x}}_{11}$	$\cdots$	$\bar{x}_{1s}$	$\hat{x}_{11}$	$\cdots$	$\hat{x}_{1s}$	
$\vdots$	$\vdots$		$\vdots$			$\vdots$			$\vdots$		
c_s	v_s	x_{s1}	$\cdots$	x_{ss}	$\bar{x}_{s1}$	$\cdots$	$\bar{x}_{s1}$	$\hat{x}_{s1}$	$\cdots$	$\hat{x}_{ss}$	(17)
		$b_1(\theta$	$\cdots$	$b_S(\theta$	$b_1(\theta$	$\cdots$	$b_S(\theta$	$b_1(\theta$	$\cdots$	$b_S(\theta$	

The order condition of the TD-MIRK methods

The order conditions of the methods in (4) and (5) are obtained by Taylor's series expansion approach about x_n and equating the power of h to zero gives stage order q

$$C = Xe + v;$$

$$\frac{c^j}{j!} = \frac{Xc^{j-1}}{(j-1)!} + \frac{\bar{X}c^{j-2}}{(j-2)!} + \frac{v}{j!} \quad j = 2, \tag{7}$$

$$\frac{c^j}{j!} = \frac{Xc^{j-1}}{(j-1)!} + \frac{\bar{X}c^{j-2}}{(j-2)!} + \frac{\bar{X}c^{j-3}}{(j-3)!} + \frac{v}{j!} \quad j = 3(1)q,$$

and the method of order p

$$b^T e = e \tag{8}$$

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

$$\frac{1}{j!} = \frac{b^T c^{j-1}}{(j-1)!} + \frac{\bar{b}^T c^{j-2}}{(j-2)!} + \frac{\bar{b}^T c^{j-3}}{(j-3)!} + \frac{v}{j!} \quad j = 3(1)$$

Stability Analysis

The stability of the method (4) and (5) is analyzed by deriving their stability function for a TD-MIRK method applied to the linear test equation $y(x)' = \lambda y(x)$, the stability function $R(z)$ is given

$$R(z) = \frac{I - zX - z^2\bar{X} - z^3\hat{X} + zeb^T + z^2\overline{eb}^T + z^3 e\hat{b}^T - zvb^T - z^2 v\bar{b}^T - z^3 v\hat{b}^T}{I - zX - z^2\overline{X - z^3\hat{X}} - zvb^T - z^2 v\bar{b}^T - z^3 v\hat{b}^T}, z = \lambda h. \tag{9}$$

we derive by considering the scalar test equation $y' = \lambda y(x)$, For this problem, the associated stage derivatives satisfy $f = \lambda y$, $g = \lambda^2 y$ and $l = \lambda^3 y$, demonstrating that each higher order stage derivative arises directly from the stage value Y through successive applications of the operator λ To simplify, we take $e = (1, \dots, 1)^T$ and $v = (v_1 \dots, v_s)^T$, Hence, (4) and (5) reduces to the form

$$\left(I - zX - z^2\bar{X} - z^3\hat{X}\right)Y - vy_{n+1} = (e - v)y_n \tag{10}$$

and

$$\left(-zb^T - z^2\bar{b}^T - z^3\hat{b}^T\right)Y + y_{n+1} = y_n \tag{11}$$

From (10) we have,

$$Y = \frac{(e-v)y_n + vy_{n+1}}{(I - zX - z^2\bar{X} - z^3\hat{X})} \tag{12}$$

Inserting (12) into (11) gives

$$\left(-zb^T - z^2\bar{b}^T - z^3\hat{b}^T\right)\left(\frac{(e-v)y_n + vy_{n+1}}{(I - zX - z^2\bar{X} - z^3\hat{X})}\right) + y_{n+1} = y_n \tag{13}$$

Multiplying both side of the (13) by $\left(I - zX - z^2\bar{X} - z^3\hat{X}\right)$ gives

$$\left(-zb^T - z^2\bar{b}^T - z^3\hat{b}^T\right)\left((e-v)y_n + vy_{n+1}\right) + \left(I - zX - z^2\bar{X} - z^3\hat{X}\right)y_{n+1} = \left(I - zX - z^2\bar{X} - z^3\hat{X}\right)y_n \tag{14}$$

Simplifying (14) and collecting like terms yields

$$\left[v\left(-zb^T - z^2\bar{b}^T - z^3\hat{b}^T\right) + \left(I - zX - z^2\bar{X} - z^3\hat{X}\right)\right]y_{n+1} = \left[\left(I - zX - z^2\bar{X} - z^3\hat{X}\right)(e-v)\left(-zb^T - z^2\bar{b}^T - z^3\hat{b}^T\right)\right]y_n. \tag{15}$$

From (15) we obtain $y_{n+1} = R(z)y_n$. Thus the stability function is

$$R(z) = \frac{I - zX - z^2\bar{X} - z^3\hat{X} + zeb^T + z^2e\bar{b}^T + z^3e\hat{b}^T - zvb^T - z^2v\bar{b}^T - z^3v\hat{b}^T}{I - zX - z^2\bar{X} - z^3\hat{X} - zvb^T - z^2v\bar{b}^T - z^3v\hat{b}^T} \tag{16}$$

Construction of the TD-MIRK method

Here, we derive the method introduced in (4) and (5) a scheme characterized with order of accuracy and stage order. Methods where p=q are highly promising for practical applications, (see [2] [9],[10],[18],[19]). we therefore restrict our analysis exclusively to this class of method. The derivation presented herein adopted an approach analogous to the ones detailed in [2], [18], and [19].

5.1. TD-MIRK method of order p=q=7, s=3

A system of linear equations was derived from (7) and (8) with p=q=7 and s=3, and solved to o btain expressions in terms of $\{c_r\}_{r=1}^{s}$ such that $c_1 = c_2 = c_3$. The Butcher tableau for the p=7 method is given by

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

c	v	X			$\bar{X}$			$\hat{X}$		
0	0	0	0	0	0	0	0	0	0	0
1	1	0	0	0	0	0	0	0	0	0
$\frac{3}{4}$	$\frac{30456}{32768}$	$\frac{924}{32768}$	$\frac{-6804}{32768}$	0	$\frac{114}{32768}$	$\frac{648}{32768}$	0	$\frac{9}{32768}$	$\frac{-27}{32768}$	0
		$\frac{2932}{7560}$	$\frac{-3564}{7560}$	$\frac{8192}{7560}$	$\frac{444}{7560}$	$\frac{756}{7560}$	0	$\frac{27}{7560}$	$\frac{-45}{7560}$	0

(17)

Method in (17) stability function is $R(z) = -\frac{3360+1560z+300z^2+28z^3+z^4}{3360-1800z+420z^2-52z^3+3z^4}$ .The boundary locus for the scheme in (17) reveals it is A-stable

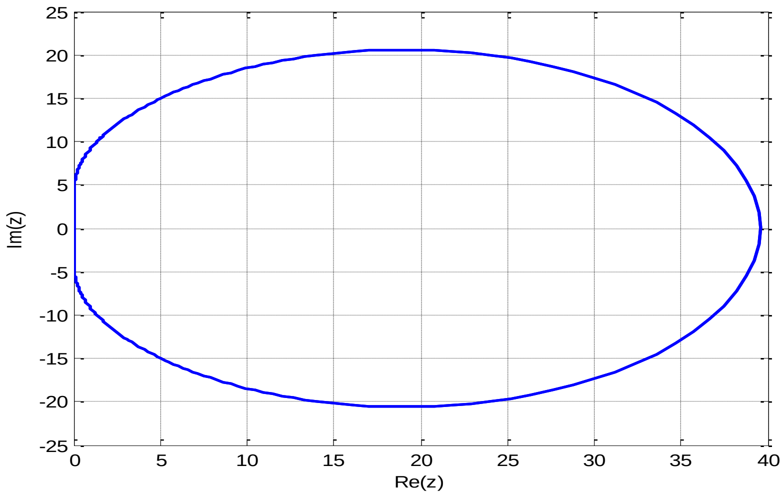

Figure1: Stability plot for TD−MIRK

5. Numerical Experiment

The performance and accuracy of theTD−MIRK7 scheme are evaluated through numerical experiments in this section

The7thorde

$$y_{n+\frac{3}{4}} = \frac{2312}{32768}y_n + \frac{30456}{32768}y_{n+1} + \frac{924h}{32768}f_n - \frac{6804h}{32768}f_{n+1} + \frac{144h^2}{32768}g_n + \frac{144h^2}{32768}g_{n+1} + \frac{9h^3}{32768}l_n - \frac{27h^3}{32768}l_{n+1}$$

$$y_{n+1} = y_n + \frac{2932h}{7560}f_n - \frac{3564h}{7560}f_{n+1} + \frac{8192h}{7560}f_{n+\frac{3}{4}} + \frac{444h^2}{7560}g_n + \frac{756h^2}{7560}g_{n+1} + \frac{27h^3}{7560}l_n - \frac{45h^3}{7560}l_{n+1}$$

We benchmark the performance of our method against those in [5], assessing accuracy on the following problems.

Problem 1: source: [5]

$$\begin{cases} y' = 198y + 199z, \\ z = -398y - 399z, \qquad , \\ y(0) = 1, \qquad z(0) = 1, \\ \text{exact solution: } y(x) = e^{-x}, z(x) = -e^{-x} \end{cases}$$

Table 1: Comparison of errors in TDMIRK7 (17) with [5] for problem 1.

	Error in [5] (p=10)		TD-MIRK 7 (P=7)	
x	y(x)	z(x)	y(x)	z(x)
0.1	8.44×10^{-9}	7.04×10^{-9}	1.30×10^{-14}	1.30×10^{-14}
0.2	1.65×10^{-8}	1.51×10^{-8}	1.27×10^{-14}	1.26×10^{-14}
0.3	2.29×10^{-8}	2.18×10^{-8}	1.29×10^{-14}	1.27×10^{-14}
0.4	2.81×10^{-8}	2.69×10^{-8}	1.28×10^{-14}	1.29×10^{-14}
0.5	3.19×10^{-8}	3.10×10^{-8}	1.87×10^{-14}	1.86×10^{-14}
0.6	3.49×10^{-8}	3.40×10^{-8}	1.58×10^{-14}	1.60×10^{-14}
0.7	3.69×10^{-8}	3.61×10^{-8}	2.56×10^{-14}	2.55×10^{-14}
0.8	3.83×10^{-8}	3.76×10^{-8}	2.95×10^{-14}	2.95×10^{-14}
0.9	3.91×10^{-9}	3.84×10^{-8}	3.11×10^{-14}	3.11×10^{-14}
1.0	3.94×10^{-8}	3.88×10^{-8}	3.45×10^{-14}	3.44×10^{-14}

Table1 established that the new method TD−MIRK7 of order7 demonstrates superior accuracy to the existing method of order10 in [5], which makes it appropriate for the integration of stiff system in ODEs.

Problem 2: source: [5]

$$\begin{cases} y' = 100y + 9.901z, \\ z = 0.1y - z, \quad , \\ y(0) = 1, \quad z(0) = 10, \\ \text{exact solution: } y(x) = e^{-\frac{99}{100}x}, z(x) = 10e^{-\frac{99}{100}x} \end{cases}$$

Table 2: Comparison of errors in TDMIRK7 (17) with [5] for problem 1.

	Error in [5] (p=10)		TD-MIRK 7 (P=7)	
x	y(x)	z(x)	y(x)	z(x)
0.1	8.85×10^{-11}	3.26×10^{-9}	7.78×10^{-15}	7.79×10^{-14}
0.2	2.14×10^{-10}	5.91×10^{-9}	1.08×10^{-14}	1.09×10^{-13}
0.3	4.62×10^{-10}	8.03×10^{-9}	1.33×10^{-14}	1.34×10^{-13}
0.4	6.61×10^{-10}	9.70×10^{-9}	1.75×10^{-14}	1.27×10^{-13}
0.5	8.18×10^{-10}	1.09×10^{-8}	1.90×10^{-14}	1.92×10^{-13}
0.6	9.04×10^{-10}	1.19×10^{-8}	2.03×10^{-14}	2.04×10^{-13}
0.7	1.03×10^{-9}	1.26×10^{-8}	2.24×10^{-14}	2.24×10^{-13}
0.8	1.09×10^{-9}	1.30×10^{-8}	2.27×10^{-14}	2.27×10^{-13}
0.9	1.14×10^{-9}	1.33×10^{-8}	2.32×10^{-14}	2.30×10^{-13}
1.0	1.16×10^{-9}	1.34×10^{-8}	2.31×10^{-14}	2.30×10^{-13}

In Table 2, for problem 2 the numerical results reveals that the TD − MIRK7 in (17) is better in terms of accuracy than method in [5] . The numerical results in Table 2 show that the new methods are capable of giving accurate and stable results, hence the TD − MIRKM7 performed better than the [5] as expected.

Conclusion

In this study, we introduce TD−MIRK method that is A-stable for the numerical treatment of stiff initial value problems in ordinary differential equations. The stability investigation presented in Section 4, along with the illustration in Figure 1, confirms that the method achieves both zero-stability and A-stability. The numerical outcomes in Tables 1 and 2 further demonstrate that the proposed approach outperforms existing techniques reported in the literature.

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