

**GENERALISED SECOND DERIVATIVE MONO
IMPLICIT RUNGE-KUTTA METHODS FOR
STIFF ORDINARY DIFFERENTIAL
EQUATIONS**

BY

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AUGUST, 2019

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**A THESIS SUBMITTED TO THE DEPARTMENT OF
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CERTIFICATION

This is to certify that this thesis was carried out and written by **Afolabi Gabriel ARIWAYO** with matriculation number **PG/PSC1614508** of the Department of Mathematics, Faculty of Physical Sciences, University of Benin, Benin City, under the supervision of Prof. R.I. Okuonghae.

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DEDICATION

This thesis is dedicated to God almighty and my late mother Princess Adetola Martha Ariwayo.

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ABSTRACT

Numerical schemes for the integration of stiff initial value problems are required to possess wide region of absolute stability which include the entire left of the complex plane. Numerical schemes that are explicit usually do not attain the requirement for integration of stiff initial value problems. In this study, implicit second derivative Runge-Kutta methods are constructed for the integration of stiff initial value problems.

A family of generalised second derivative mono-implicit Runge-Kutta (GSDMIRK) method is derived using the method of Tailor series expansion.

The proposed GSDMIRK methods are A -stable for stage $s=3$ and 4 and $A(\infty)$ -stable for $s=5$ and 6. Numerical experiments show that the GSDMIRK methods perform better when compared to some numerical algorithms in the literature.

CHAPTER ONE

INTRODUCTION

1.1 Background of the study

The translation of some real life situations to mathematical models often lead to differential equations (DEs). Examples are determination of motion of planetary bodies, rate of decay of radioactive elements and change in population over a period of time, Burrage (1994). Mathematical models often give rise to DEs 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).

This study is organized as follows; in this chapter, we give summary of different types of differential equations and also discuss stiffness of DEs. Chapter Two describes Runge-Kutta (RK) methods and Mono-implicit Runge-Kutta methods (MIRK) to introduce second derivative MIRK methods. The order and stage order for a MIRK method are explained, and we give examples of MIRK methods having orders 1 through 6. In Chapter three, we carry out the derivation of our proposed generalized second derivative mono implicit Runge-Kutta methods (GSDMIRK) methods for stiff ODEs. Chapter Four discusses the stability analysis of the generalized SDMIRK methods. In Chapter five, we focus on the implementation strategies and results obtained from numerical experiments by comparing the proposed GSDMIRK methods with other existing methods in the literature. Also Chapter Five gives the summary and conclusion of the work.

1.2 Ordinary Differential Equations

An ordinary differential equation (ODE) is an equation that includes a function of one independent variable x (e.g, time or space) and derivatives of this function with respect to x , Ascher *et. al* (1995).

In this study, we assume a system of ODEs having the general form

$$y'(x) = f(x, y(x)), y: R \rightarrow R^n, f: R \times R^n \rightarrow R^n \quad (1.2.1)$$

where y and f are vector functions of dimension n .

ODEs occur in many applications, these include, for instance, modelling of human heart, the spread and control of diseases (or viruses), Ascher *et. al* (1995).

1.2.1 Initial Value and Boundary Value ODEs

An ordinary differential equation (1.2.1) together with an initial condition

$$y(a) = y_0 \quad (1.2.2)$$

is called an initial value ODE, where a and y_0 are given values. The initial condition (1.2.2) is used to determine the value of the integration constant appearing in the general solution of (1.2.1), Ascher *et. al* (1995).

Boundary value ODEs (BVODEs) are systems of differential equations for which the values of the solution components are specified at two distinct points, Ascher *et. al* (1995). We are interested in the BVODEs written in first order system of (1.2.1) with boundary conditions (BCs)

$$g(y(a), y(b)) = 0 \quad (1.2.3)$$

where $g: R^n \times R^n \rightarrow R^n$ is a vector function, and $0 \in R^n$ is the zero vector.

1.2.2 Stiff ODEs

There are different definitions of stiff ODEs in the literature. Stiffness in differential equations was first observed by two chemists; Curtiss and Hirschfelder in 1952. They gave the definition of stiffness as follows: “stiff equations are equations where certain implicit methods perform better, usually tremendously better, than explicit ones” Butcher (1964). The next important development was by Dahlquist, see Dahlquist (1963). From his work, he defined stiff ODE systems as “systems containing very fast components as well as slow components”.

Stiff differential equations are problems for which explicit methods do not work, hence implicit methods are highly recommended for stiff ODEs. The most common phenomena that describe stiffness is when the eigenvalues of the Jacobian of the system of ODEs differs greatly in magnitude, Henrici, (1962). In the course of obtaining solutions to these ODEs, some of the ODEs cannot be solved analytically, hence approximate numerical solutions are essential. The first numerical methods to be proposed for integrating stiff initial value problems (IVPs) is the Backward Differentiation Formula (BDF) as noted in the pioneering work of Curtiss and Hirschfelder (1952).

The chemical reaction of Robertson is one of the most well-known examples that involve stiff ODEs. The equations and initial values are given by, see Horn (1982)

$$y'_1 = -0.04y_1 + 10^4 y_2 y_3, \quad y_1(0) = 1 \quad (1.2.4)$$

$$y'_2 = 0.04 y_1 - 3.10^7 y_2 y_3, \quad y_2(0) = 0 \quad (1.2.5)$$

$$y'_3 = 3 \times 10^7 y_2^2, \quad y_3(0) = 0 \quad (1.2.6)$$

where the reaction rate 0.04 is relatively slow, while the reaction rate 3.0×10^7 is very fast.

1.3 Statement of Problem

Over the years, the development of numerical schemes for the solution of IVPs in ODEs has been an area of interest to researchers, especially ODEs that arise from modeling real life situations. But the problem with some of these numerical schemes is their inability to properly solve stiff ODEs due to their small region of absolute stability. Hence the need for the development and modification of numerical schemes with wide region of absolute stability suitable for the solution of stiff ODEs. In the spirit of this, this study proposes a family GSDMIRK methods with good stability properties.

1.4 Aim and Objectives

The aim of this study is to develop a new family of GSDMIRK methods that possess high order and good stability properties for the solution of system of IVPs (1.2.1) of stiff ODEs.

The primary objectives with respect to this aim are to:

1. determine the stability properties of the proposed GSDMIRK methods
2. present numerical results from the schemes on some stiff test problems

1.5 Methodology

In this study, we are interested in the development of the generalized second derivative mono implicit Runge-Kutta methods. Taylor series expansion is employed for the derivation of the proposed GSDMIRK methods. Our proposed method is in the spirit of mono implicit Runge-Kutta (MIRK) methods developed by Dow (2017).

CHAPTER TWO

RUNGE-KUTTA METHODS

2.1 Introduction

The Runge-Kutta (RK) method was first proposed by Carl Runge in 1895, further contributions were made by Heun and Martin in 1900 and 1901 respectively, Butcher (1964). Detailed history of RK methods is in Butcher (1964). RK method is used for the numerical approximation of ODEs (1.2.1). The general form of RK method according to Lambert (1973) is

$$y_{n+1} = y_n + h \sum_{r=1}^s b_r k_r, \quad (2.1.1)$$

here s indicates the number of stages of the process and h is the step size. The stages k_r are defined by

$$k_r = f \left(x_r + c_r h, y_n + \sum_{j=1}^s a_{rj} k_j \right), r = 1(1)s \quad (2.1.2)$$

with constraint

$$\sum_{r=1}^s b_r = 1 \quad (2.1.3)$$

and

$$c_r = \sum_{j=1}^s a_{rj}, r = 1(1)s \quad (2.1.4)$$

For an Explicit RK method, (2.1.2) takes the form

$$k_r = f \left(x_r + c_r h, y_n + \sum_{j=1}^{s-1} a_{rj} k_j \right), r = 1(1)s \quad (2.1.5)$$

The coefficients $\{a_{rj}, b_r, c_r\}$ for the algorithms in (2.1.1) and (2.1.2) can be represented on a Butcher tableau as follows

c_1	a_{11}	a_{12}	\cdots	a_{1s}
\vdots	a_{21}	a_{22}	\cdots	a_{2s}
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	\cdots	a_{ss}
	b_1	b_2	\cdots	b_s

The compact form of the above tableau is given as

c	A
	b^T

In (2.1.1) and (2.1.2) the components of the $A = (a_{rj})$ matrix are the coefficients used to find the internal stages using linear combinations of the stages derivatives, and A is an s by s matrix whose (r, j) th component is a_{rj} , and $b = (b_1, b_2 \cdots, b_s)^T$ is the vector of weights indicating how the approximation to the solution depends on the derivatives of the internal stages and $c = (c_1, c_2 \cdots, c_s)^T$, is the abscissae vector representing the position of the approximation in the step while $e = (1, \cdots, 1)^T$ (that is, e is the vector of 1's of length s). In this general formulation k_r represents the internal stage values

and y_n is the numerical approximation to the solution $y(x_n)$ and stage derivatives is $\{f(k_r)\}_{r=1}^s$.

The RK method (2.1.1) is divided into explicit and implicit methods. The first is easy and has cheap implementation cost but has limited region of absolute stability thus not suitable for the numerical solution of (1.2.1) if stiff. The latter is expensive and difficult to implement but is known for large interval of absolute stability property and suitable for stiff IVPs in (1.2.1), Abdi and Hojjati (2011), Aiguobasimwin (2019), Ascher *et. al*, (1995), Burrage *et. al* (1994), Butcher (1964), Butcher (1997), Butcher (2005) and Butcher (2016).

2.2 Explicit Runge-Kutta (ERK) Method

A RK method (2.1.1) is explicit if $a_{rj} = 0; j \geq r$ (that is, A is lower triangular matrix with zero diagonal elements).

The Butcher tableau for ERK methods is

c_1	0	0	...	0
\vdots	a_{21}	0	...	0
\vdots	\vdots	\vdots	\ddots	\vdots
c_s	a_{s1}	a_{s2}	...	0
	b_1	b_2	...	b_s

A method for the direct solution of (1.2.1) is the Almost Runge-Kutta (ARK) method. This method was first introduced by Butcher (1997). In that paper, the author considered an explicit ARK methods of order two up to four. The beauty about this method is that it shares the same stability function with the well-known RK method and with such characteristics, the method behaves exactly like RK method. Butcher (1998) again show how to obtain an explicit ARK method of order five via an algebraic and B-series approach. In the spirit of Butcher (1998), Butcher and Rattenbury (2005) introduced ARK method for the solution of stiff ODEs.

Recently Chan and Tsai (2010) introduced explicit two-derivative version of the RK (ETDRK) method. The order conditions of the ETDRK method were derived using the rooted tree approach, see Butcher (1997).

The simplest explicit RK (ERK) method is the Euler method, Butcher (2016). The formula for this method is

$$y_{n+1} = y_n + hf(x_n, y_n) \tag{2.2.6}$$

The Butcher tableau for (2.2.5) is

0	0
	1

The explicit Euler method is of order 1.

Example of ERK method is the explicit 3-stage RK method, Butcher (2016) and is given as

$$y_{n+1} = y_n + \frac{h}{4}(k_1 + 3k_3) \tag{2.2.7}$$

where

$$k_1 = f(x_n, y_n),$$

$$k_2 = f\left(x_n + \frac{h}{3}, y_n + \frac{h}{3}k_1\right), \quad k_3 = f\left(x_n + \frac{2h}{3}, y_n + \frac{2h}{3}k_2\right).$$

The Butcher tableau of the RK method in (2.2.7) is

0	0	0	0
$\frac{1}{3}$	$\frac{1}{3}$	0	0
$\frac{2}{3}$	0	$\frac{2}{3}$	0
	$\frac{1}{4}$	0	$\frac{3}{4}$

Example of an explicit RK method is the 4-stage RK method Butcher (1987) and is given an

$$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{2.2.8}$$

where

$$k_1 = f(x_n, y_n), \quad k_2 = f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_1\right),$$

$$k_3 = f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_2\right), \quad k_4 = f(x_n + h, y_n + hk_3).$$

and its tableau is given by

0	0	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0	0
$\frac{1}{2}$	0	$\frac{1}{2}$	0	0
1	0	0	1	0
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

2.3 Implicit Runge-Kutta (IRK) Method

The RK method in (2.1.1) is fully implicit if $a_{rj} \neq 0$ for at least one $j > r$. The Butcher tableau of this type of RK method is

c_1	a_{11}	\cdots	a_{1s}
\vdots	\vdots		\vdots
c_s	a_{s1}	\cdots	a_{ss}
	b_1	\cdots	b_s

An example of IRK method is the 2-stage order 4 IRK method (Gauss method), Butcher (2016)

This method is given as

$$y_{n+1} = y_n + \frac{h}{2}(k_1 + k_2) \tag{2.3.9}$$

where

$$k_1 = f\left[x_n + \frac{h}{2}\left(1 - \frac{\sqrt{3}}{3}\right), y_n + \frac{h}{4}k_1 + \frac{h}{2}\left(\frac{1}{2} - \frac{\sqrt{3}}{3}\right)k_2\right],$$

$$k_2 = f\left[x_n + \frac{h}{2}\left(1 + \frac{\sqrt{3}}{3}\right), y_n + \frac{h}{2}\left(\frac{1}{2} + \frac{\sqrt{3}}{3}\right)k_1 + \frac{h}{4}k_2\right].$$

The tableau of this method is given as

$\frac{1}{2} - \frac{\sqrt{3}}{6}$	$\frac{1}{4}$	$\frac{1}{4} - \frac{\sqrt{3}}{6}$
$\frac{1}{2} + \frac{\sqrt{3}}{6}$	$\frac{1}{4} + \frac{\sqrt{3}}{6}$	$\frac{1}{4}$
	$\frac{1}{2}$	$\frac{1}{2}$

An example of IRK method is the 2-stage order 3 RK method (Radau IIA), Butcher (2016).

This method is given as

$$y_{n+1} = y_n + \frac{h}{4}(3k_1 + k_2) \tag{2.3.10}$$

where

$$k_1 = f\left(x_n + \frac{h}{3}, y_n + \frac{h}{12}(5k_1 - k_2)\right)$$

$$k_2 = f\left(x_n + h, y_n + \frac{h}{4}(3k_1 + k_2)\right)$$

The Butcher Tableau of this method is

$\frac{1}{3}$	$\frac{5}{12}$	$\frac{-1}{12}$
$\frac{1}{3}$	$\frac{3}{4}$	$\frac{1}{4}$
1	$\frac{3}{4}$	$\frac{1}{4}$

For IRK methods, each stage k_r in (2.2.1) is implicitly defined in terms of itself and other stages. Therefore, to compute values for the stages, it is essential to solve non-linear system of dimension $n \times s$ where n represents the number of DEs and s represents number of stages of the method. The non-linear system for the determination of the stages is often solved using a Newton type iteration which makes the calculation of the stages a computationally expensive process, Butcher (1987).

In the spirit of Dalhquist (1963), Ehle in 1969 shows that the implicit RK method derived by Butcher (1963) and Butcher (1964) has large interval of absolute stability,

therefore suitable for the numerical solution of stiff IVPs in (1.2.1). One practical disadvantage associated with an IRK method is the computational cost of solving a system of nonlinear implicit equations. More examples of IRK methods can be found in the work of Abdi and Hojjti (2011), Butcher (1963), Butcher (1964), Butcher (2005), Butcher (1977), Butcher (2016), Fatunla (1978), Hairer and Wanner (1996), Mehdizadeh (2015), Vigo-Aguiar and Ramos (2007).

In 2014, Tsai *et. al* (2014) introduced an implicit counter part of the two-derivative RK (TDIRK) method. Okuonghae and Ikhile (2014) use collocation approach to obtain L -stable TDIRK methods of order four, five and six respectively. It is found in the literature that subclasses of the TDIRK methods exist, see Mitsui (1982) and Muir and Enright (1987).

A slight modification of RK method in (2.1.1) results to the two-step RK (TSRK) methods, a method introduced in Jackiewicz *et. al* (1991). The authors derive the order conditions of the TSRK method via Taylor series expansion. Other subclasses of the TSRK methods are in Faragó (2013), Jackiewicz and Tracogna (1995), Jackiewicz *et. al* (1995), Jackiewicz and Verner (2002), Jackiewicz (2009). The two-derivative version of the TSRK methods in Jackiewicz *et. al* (1991) can be found in Aiguobasimwin (2019), Turaci and Ozi (2018) and Okuonghae and Aiguobasimwin (2017).

For example, an IRK method having order 1, must satisfy

$$b^T e = 1 \tag{2.3.11}$$

The order condition for second order is

$$b^T e = \frac{1}{2} \tag{2.3.12}$$

An IRK method must satisfy (2.3.11) and (2.3.12) in order to be second order.

The order conditions for third order are

$$b^T c^2 = \frac{1}{3}, b^T A c = \frac{1}{6} \quad (2.3.13)$$

where $c^j = (c_1^j, c_2^j, \dots, c_s^j)^T$.

An IRK method must satisfy (2.3.11), (2.3.12) and (2.3.13) before it can be of the third order. Fourth order has the following order conditions:

$$b^T c^3 = \frac{3}{4}, b^T c A c = \frac{1}{8}, b^T A c^2 = \frac{1}{12}, b^T A^2 c = \frac{1}{24} \quad (2.3.14)$$

So, for an IRK method to be fourth order it must satisfy all conditions of (2.3.11), (2.3.12), (2.3.13) and (2.3.14).

2.4 Semi Implicit Runge-Kutta (SIRK) Method

Subclass of IRK method is the so-called semi implicit RK method. The RK method in (2.1.1) is semi implicit if $a_{rj} = 0; j > r$ (that is, A is a lower triangular matrix with non-zero diagonal elements). This method is also known as diagonal implicit RK (DIRK) method. The tableau for this method is

c_1	a_{11}	0	\dots	0
\vdots	a_{21}	\ddots	\dots	0
\vdots	\vdots	\ddots	\vdots	\vdots
c_s	a_{s1}	\dots	\dots	a_{ss}
	b_1	\dots	\dots	b_s

The following are the examples of semi implicit RK methods:

Implicit midpoint rule, Butcher (2016)

This method is given as

$$y_{n+1} = y_n + \frac{h}{2}k_1 \quad (2.4.15)$$

where

$$k_1 = f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}k_1\right)$$

The tableau of this method is as follows

$\frac{1}{2}$	$\frac{1}{2}$
	$\frac{1}{2}$

2-stages order 2 semi IRK method, Butcher (2016).

This method is given as

$$y_{n+1} = y_n + h \left[\frac{\sqrt{2}}{2}k_1 + \left(1 - \frac{\sqrt{2}}{2}\right)k_2 \right] \quad (2.4.16)$$

where

$$k_1 = f\left[x_n + h\left(1 - \frac{\sqrt{2}}{2}\right), y_n + \left(1 - \frac{\sqrt{2}}{2}\right)k_1\right],$$

$$k_2 = f\left[x_n + h, y_n + \frac{\sqrt{2}}{2}k_1 + \left(1 - \frac{\sqrt{2}}{2}\right)k_2\right].$$

Its tableau is represented as follows

$$\begin{array}{c|cc}
1 - \frac{\sqrt{2}}{2} & 1 - \frac{\sqrt{2}}{2} & 0 \\
1 & \frac{\sqrt{2}}{2} & 1 - \frac{\sqrt{2}}{2} \\
\hline
& \frac{\sqrt{2}}{2} & 1 - \frac{\sqrt{2}}{2}
\end{array}$$

2.5 Stability of Runge-Kutta Method

To determine the region of absolute stability of the RK method in (2.1.1) we applied the RK method in (2.1.1) to the scalar test equation

$$y' = \lambda y, \quad Re(\lambda) < 0 \quad (2.5.17)$$

and obtained

$$y_{n+1} = (1 + zb^T(I - zA)^{-1}e)y_n, \quad (z = \lambda h) \quad (2.5.18)$$

where I is an $s \times s$ identity matrix, $A = (a_{rj})$ an $s \times s$ matrix and $e = (1, \dots, 1)^T$.

Therefore the stability function $R(z)$ of an s -stage RK method is given by

$$R(z) = 1 + zb^T(1 - zA)^{-1}e. \quad (2.5.19)$$

2.6 Mono-Implicit Runge-Kutta Methods (MIRK)

In this study, our interest is on the extension (second derivative) of mono-implicit RK (MIRK) method for the numerical solution of (1.2.1). The MIRK formula was introduced by Muir and Enright (1987). The general form of MIRK method is

$$y_{n+1} = y_n + h \sum_{r=1}^s b_r k_r \quad (2.6.20)$$

where

$$k_r = f \left((1 - v_r)y_n + v_r y_{n+1} + h \sum_{j=1}^{r-1} X_{rj} k_j \right), r = 1(1)s \quad (2.6.21)$$

s indicates the number of stages, the coefficients of (2.6.20) and (2.6.21) are $\{v_r\}_{r=1}^s$ and $\{x_{rj}\}_{j=1, r=1}^{r-1}$, and the weights are $\{b_r\}_{r=1}^s$. The abscissa, $\{c_r\}_{r=1}^s$, are defined by the following equation

$$c_r = v_r + \sum_{j=1}^{r-1} X_{rj} \quad (2.6.22)$$

As RK methods are being represented in Butcher tableau [see sec. (2.1)], also MIRK methods can be represented in the Butcher tableau of the form

c_1	v_1	0	0	0	0
c_2	v_2	x_{21}	0	0	0
\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
\vdots	\vdots	\vdots	\ddots	\vdots	\vdots
c_s	v_s	x_{s1}	x_{s2}	$x_{s,s-1}$	0
		b_1	b_2	b_s	

which can sometimes be condensed to

\mathbf{c}	\mathbf{v}	X
		\mathbf{b}^T

where $c = (c_1, c_2, \dots, c_s)^T$, $v = (v_1, v_2, \dots, v_s)^T$, $b = (b_1, b_2, \dots, b_s)^T$, X is an $s \times s$ matrix whose (r, j) th components is x_{rj} . X is strictly lower triangular matrix. Examples of MIRK method is in Burrage *et. al* (1994), Capper and Moore (2006), De Meyer *et. al* (1997), Dow (2017), Muir and Enright (1987), Muir and Owren (1993), Muir and Adams (2001). The advantage of MIRK methods (2.6.20) is that, its implementation attracts low computational cost in term of the number of nonlinear equations to be solved. For MIRK methods (2.6.20), all stages k_r are implicit only in y_{n+1} , Muir and Owren (1993).

2.7 Order Conditions and Local Truncation Error for MIRK Methods

The order condition of RK methods are usually obtained via Taylor series expansion Lambert (1973), B-series of Butcher, Jackson (1994), the Butcher rooted tree in Butcher (2009) and the collocation and interpolation scheme in Harrier, wanner and Nosette (1987), Okuonghae (2013), Okuonghae (2014), Okuonghae and Ikhile (2014), Onumanyi *et. al* (2012), e.t.c. In this study, we are interested in determining the order conditions via Taylor series expansion as follows:

the local truncation error of (2.6.21) is given as

$$L_s(y(x); h) = y(x_n + c_r h) - [(1 - v_r)y(x_n) + v_r y(x_n + h) + h \sum_{j=1}^{r-1} X_{rj} y'(x_n + c_r h)] \quad (2.7.23)$$

Expanding (2.7.23) by Taylor series about x_n yields

$$L_s(y(x); h) = C_0 y(x_n) + C_1 h y'(x_n) + C_2 h^2 y''(x_n) + \dots + C_p h^p y^{(p)}(x_n) + C_{p+1} h^{p+1} y^{(p+1)}(x_n) \quad (2.7.24)$$

where

$$C_1 = c_r - v_r - \sum_{j=1}^{r-1} X_{rj} = 0$$

$$C_2 = \frac{1}{2}(c_r^2 - v_r) - \sum_{j=1}^{r-1} c_j X_{rj} = 0$$

$$C_3 = \frac{1}{3!}(c_r^3 - v_r) - \frac{1}{2} \sum_{j=1}^{r-1} c_j^2 X_{rj} = 0$$

$$C_4 = \frac{1}{4!}(c_r^4 - v_r) - \frac{1}{3!} \sum_{j=1}^{r-1} c_j^3 X_{rj} = 0$$

⋮ ⋮ ⋮

$$C_q = \frac{1}{q!}(c_r^q - v_r) - \frac{1}{(q-1)!} \sum_{j=1}^{r-1} c_j^{q-1} X_{rj} = 0$$

hence the stage error constant is

$$C_{q+1} = \frac{1}{(q+1)!}(c_r^{q+1} - v_r) - \frac{1}{q!} \sum_{j=1}^{r-1} c_j^q X_{rj} \quad (2.7.25)$$

where $C_{q+1} \neq 0$ and q is the stage order.

From (2.7.25) a MIRK method is of stage order q if its coefficients satisfy (2.7.26)

$$\frac{Xc^{j-1}}{(j-1)!} + \frac{v}{j!} = \frac{c^j}{j!}, \quad j = 1, 2, \dots, q \quad (2.7.26)$$

Similarly, for the output method in (2.6.20), the local truncation error is given as

$$L_S(y(x); h) = y(x_n + c_r h) - [y(x_n) + h \sum_{r=1}^s b_r y'(x_n + c_r h)] \quad (2.7.27)$$

Expanding (2.7.27) by Taylor series about x_n yields

$$L_S(y(x); h) = C_0^* y(x_n) + C_1^* h y'(x_n) + C_2^* h^2 y''(x_n) + \cdots + C_p^* h^p y^{(p)}(x_n) + C_{p+1}^* h^{p+1} y^{(p+1)}(x_n) \quad (2.7.28)$$

where

$$C_1^* = 1 - \sum_{r=1}^s b_r = 0$$

$$C_2^* = \frac{1}{2} - \sum_{r=1}^s b_r c_r = 0$$

$$C_3^* = \frac{1}{3!} - \frac{1}{2} \sum_{r=1}^s b_r c_r^2 = 0$$

$$\vdots \quad \vdots \quad \vdots$$

$$C_p^* = \frac{1}{p!} - \frac{1}{(p-1)!} \sum_{r=1}^s b_r c_r^{p-1} = 0$$

The error constant for the output method is

$$C_{p+1}^* = \frac{1}{(p+1)} - \frac{1}{p!} \sum_{r=1}^s b_r c_r^p \neq 0 \quad (2.7.29)$$

where $C_{p+1}^* \neq 0$ and p is the output order.

From (2.7.29) a MIRK method is of order p if its coefficients satisfy () below

$$\frac{bc^{j-1}}{(j-1)!} = \frac{1}{j!}, \quad j = 1, 2, \dots, p \tag{2.7.30}$$

where $e = (1, 1, \dots, 1)^T$

The following examples show different MIRK methods of different orders

(a) MIRK method of order one

An example of first order, 1-stage, stage order 1 MIRK method is the explicit Euler method. The explicit Euler method has $c_1 = v_1 = 0$ and $b_1 = 1$.

c_1	v_1	0
		b_1

This class of methods also includes the first order implicit Euler method, obtained by choosing $c_1 = v_1 = 1$ and $b_1 = 1$, this method has stage order 1.

(b) MIRK method of order two

An example of a MIRK method of order 2 with 2 stages and having stage order 2 is the trapezoidal method, Burrage *et. al* (1994) with the following tableau

0	0	0	0
1	1	0	0
		$\frac{1}{2}$	$\frac{1}{2}$

(c) A MIRK Method of Order Three

An example of a 2-stage, order 3, stage order 2 MIRK method, Burrage *et. al* (1994) is

1	1	0	0
$\frac{1}{3}$	$\frac{5}{9}$	$\frac{-2}{9}$	0
		$\frac{1}{4}$	$\frac{3}{4}$

(d) A MIRK Method of Order Four

A unique MIRK method of 3-stage, order 4, stage order 3 is represented in the following tableau, Burrage *et. al* (1994)

0	0	0	0	0
1	1	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{8}$	$\frac{-1}{8}$	0
		$\frac{1}{6}$	$\frac{1}{6}$	$\frac{2}{3}$

(e) A MIRK Method of Order Five

An example of a 4-stage, order 5, stage order 3 MIRK method, Burrage *et. al* (1994) is

0	0	0	0	0	0
1	1	0	0	0	0
$\frac{1}{4}$	$\frac{5}{32}$	$\frac{9}{64}$	$\frac{-3}{64}$	0	0
$\frac{7}{10}$	$\frac{413}{1250}$	$\frac{-63}{500}$	$\frac{-21}{1000}$	$\frac{252}{625}$	0

$$\frac{1}{14} \quad \frac{5}{54} \quad \frac{32}{81} \quad \frac{250}{567}$$

(f) A MIRK Method of Order Six

An example of a 5-stage, order 6 MIRK method, Burrage *et. al* (1994) is

0	0	0	0	0	0	0
1	1	0	0	0	0	0
$\frac{1}{2} - \frac{\sqrt{21}}{14}$	$\frac{1}{2} - \frac{9\sqrt{21}}{98}$	$\frac{1}{14} + \frac{\sqrt{21}}{98}$	$-\frac{1}{14} + \frac{\sqrt{21}}{98}$	0	0	0
$\frac{1}{2} + \frac{\sqrt{21}}{14}$	$\frac{1}{2} + \frac{9\sqrt{21}}{98}$	$\frac{1}{14} - \frac{\sqrt{21}}{98}$	$-\frac{1}{14} - \frac{\sqrt{21}}{98}$	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	$\frac{-5}{128}$	$\frac{5}{128}$	$\frac{7\sqrt{21}}{128}$	$-\frac{7\sqrt{21}}{128}$	0
		$\frac{1}{20}$	$\frac{1}{20}$	$\frac{49}{180}$	$\frac{49}{180}$	$\frac{16}{45}$

CHAPTER THREE

GENERALIZED SECOND DERIVATIVE MONO IMPLICIT RUNGE-KUTTA METHOD

3.1 Introduction

In this study, the focus is on the generalized second derivative mono-implicit Runge-Kutta (GSDMIRK) methods a subclass of the well-known implicit Runge-Kutta methods, Butcher (1964). An essential property of GSDMIRK method is its order; a GSDMIRK method is of order p if its global error behaves like $O(h^p)$ (the global error of a point is the difference between the numerical solution approximation at x and the exact solution at x). In this study, q is the stage order of the method while p is the order of the output method.

In this chapter, we present a family of the general structure of the generalized second derivative version of MIRK method in (2.6.20) as

$$y_{n+1} = y_n + h \sum_{r=1}^s b_r F(Y_r) + h^2 \sum_{r=1}^s \bar{b}_r \bar{F}(Y_r) \quad (3.1.1)$$

where Y_r is the stages and it is given as

$$Y_r = (1 - v_r)y_n + v_r y_{n+1} + h \sum_{i=1}^{r-1} X_{ri} F_i + h^2 \sum_{i=1}^{r-1} \bar{X}_{ri} \bar{F}_i, r = 1(1)s \quad (3.1.2)$$

Here, s represents the number of stages, the coefficients are $\{v_r\}_{r=1}^s$, $\{x_{ri}\}_{i=1,r=1}^{r-1,s}$, $\{\bar{x}_{ri}\}_{i=1,r=1}^{r-1,s}$ and $\{b_r\}_{r=1}^s$ is the weights and h is the step size. The stage values is

$$Y_r = y(x_n + c_r h); r = 1(1)s$$

where h is the step size and the abscissa vector is given as

$$c = v_r + \sum_{i=1}^{r-1} X_{ri} + \sum_{i=1}^{r-1} \bar{X}_{ri} \tag{3.1.3}$$

The Butcher's tableau format for the method (3.1.1) is

c_1	v_1	0	$0 \dots \dots \dots 0$	0	$0 \dots \dots \dots 0$
c_2	v_2	x_{21}	$0 \dots \dots \dots 0$	\bar{x}_{21}	$0 \dots \dots \dots 0$
\vdots	\vdots	$\vdots \searrow$	\vdots	$\vdots \searrow$	\vdots
\vdots	\vdots	\vdots	\searrow	\vdots	\vdots
\vdots	\vdots	\vdots	\searrow	\vdots	\vdots
c_s	v_s	x_{s1}	$x_{s2} \dots \dots \dots x_{s,s-1} 0$	\bar{x}_{s1}	$\bar{x}_{s2} \dots \dots \dots \bar{x}_{s,s-1} 0$
		b_1	$b_2 \dots \dots \dots b_s$	\bar{b}_1	$\bar{b}_2 \dots \dots \dots \bar{b}_s$

The compact of the above tableau is

c	v	X	\bar{X}
		b^T	\bar{b}^T

where

$$c = (c_1, c_2 \dots \dots c_s)^T, v = (v_1, v_2 \dots \dots v_s)^T, b = (b_1, b_2 \dots \dots b_s)^T, \bar{b} = (\bar{b}_1, \bar{b}_2 \dots \dots \bar{b}_s)^T,$$

X is the s by s matrix whose (i, j) th component is x_{ij} , and \bar{X} is the s by s matrix whose (i, j) th component is \bar{x}_{ij}

3.2 The Order Conditions for GSDMIRK Method

Additional set of conditions that can be imposed on the coefficients of GSDMIRK method are the stage order conditions. Imposing stage order conditions is often helpful, this is because it reduces the number of order conditions that must be satisfied, Okuonghae and Aiguobasimwim (2017). A GSDMIRK method is of stage order q if its coefficients satisfy the stage order conditions up to stage order q , which is represented by the following equations;

$$Xe + v = c, \quad j = 1 \tag{3.2.4}$$

$$\frac{Xc^{j-1}}{(j-1)!} + \frac{\bar{X}c^{j-2}}{(j-2)!} + \frac{v}{j!} = \frac{c^j}{j!}, \quad j = 2, \dots, q \tag{3.2.5}$$

where $e = (1, 1, \dots, 1)^T$

Also, a GSDMIRK method is of order p if its coefficients satisfy the order conditions up to order p , which is represented as

$$b^T e = e, \quad j = 1 \tag{3.2.6}$$

$$\frac{bc^{j-1}}{(j-1)!} + \frac{\bar{b}c^{j-2}}{(j-2)!} = \frac{1}{j!}, \quad j = 2, \dots, p \tag{3.2.7}$$

In the following, we will derive generalized GSDMIRK methods of orders 6, 7, 9, and 11. The MATHEMATICA software is used in the derivation of generalized SDMIRK methods.

3.3 A 3-stage, stage order 6, 6th order Generalised SDMIRK Method

The tableau of a 3-stage, stage order 6, 6th order generalized GSDMIRK method is represented as follows;

Tableau 1

0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0
c_3	v_3	x_{31}	x_{32}	x_{33}	\bar{x}_{31}	\bar{x}_{32}	\bar{x}_{33}
		b_1	b_2	b_3	\bar{b}_1	\bar{b}_2	\bar{b}_3

Fixing $p = q = 6$ in (3.2.5) and (3.2.7) gives the order conditions of GSDMIRK in (3.1.1) and (3.1.2) as

$$\begin{aligned}
 Xe + v = c; \quad Xc + \bar{X}e + \frac{v}{2} = \frac{c^2}{2}; \quad \frac{Xc^2}{2} + \bar{X}c + \frac{v}{6} = \frac{c^3}{6}; \quad \frac{Xc^3}{6} + \frac{\bar{X}c^2}{2} + \frac{v}{24} = \frac{c^4}{24}; \quad \frac{Xc^4}{24} + \frac{\bar{X}c^3}{6} + \\
 \frac{v}{120} = \frac{c^5}{120}; \quad \frac{Xc^5}{120} + \frac{\bar{X}c^4}{24} + \frac{v}{720} = \frac{c^6}{720}
 \end{aligned} \tag{3.3.8}$$

and

$$\begin{aligned}
 b^T e = 1; \quad b^T c + b^T e = \frac{1}{2}; \quad b^T c^2 + 2\bar{b}^T c = \frac{1}{3}; \quad b^T c^3 + 3\bar{b}^T c^2 = \frac{1}{4}; \quad b^T c^4 + 4\bar{b}^T c^3 = \\
 \frac{1}{5}; \quad b^T c^5 + 5\bar{b}^T c^4 = \frac{1}{6}
 \end{aligned} \tag{3.3.9}$$

respectively. Solving the order conditions in (3.3.8) and (3.3.9) and Setting $c_3 = \frac{4}{5}$ with $c_3 \neq (0,1)$, we have the following tableau:

Tableau 2

0	0	0	0	0	0	0	0	0
1	1	0	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
		$\frac{46609}{101250}$	$\frac{4297}{7986}$	$\frac{107648}{67381875}$	$\frac{901}{13500}$	$\frac{-797}{7260}$		$\frac{-416}{408375}$

3.4 A 4-Stage, stage order 7, 7th order Generalised SDMIRK Method

We represent a 4-stage, stage order 7, 7th order generalized GSDMIRK method in the following tableau:

Tableau 3

0	0	0	0	0	0	0	0	0	0
1	1	0	0	0	0	0	0	0	0
c_3	v_3	x_{31}	x_{32}	x_{33}	0	\bar{x}_{31}	\bar{x}_{32}	\bar{x}_{33}	0
c_4	v_4	x_{41}	x_{42}	x_{43}	0	\bar{x}_{41}	\bar{x}_{42}	\bar{x}_{43}	05
		b_1	b_2	b_3	b_4	\bar{b}_1	\bar{b}_2	\bar{b}_3	\bar{b}_4

Setting $p = q = 7$ in (3.2.5) and (3.2.7) gives the order conditions of GSDMIRK in (3.1.1) and (3.1.2) as

$$Xe + v = c; Xc + \bar{X}e + \frac{v}{2} = \frac{c^2}{2}; \frac{Xc^2}{2} + \bar{X}c + \frac{v}{6} = \frac{c^3}{6}; \frac{Xc^3}{6} + \frac{\bar{X}c^2}{2} + \frac{v}{24} = \frac{c^4}{24}; \frac{Xc^4}{24} + \frac{\bar{X}c^3}{6} + \frac{v}{120} = \frac{c^5}{120}; \frac{Xc^5}{120} + \frac{\bar{X}c^4}{24} + \frac{v}{720} = \frac{c^6}{720}; \frac{Xc^6}{720} + \frac{\bar{X}c^5}{120} + \frac{v}{5040} = \frac{c^7}{5040} \quad (3.4.10)$$

and

$$b^T e = 1; b^T c + b^T e = \frac{1}{2}; b^T c^2 + 2\bar{b}^T c = \frac{1}{3}; b^T c^3 + 3\bar{b}^T c^2 = \frac{1}{4}; b^T c^4 + 4\bar{b}^T c^3 = \frac{1}{5}; b^T c^5 + 5\bar{b}^T c^4 = \frac{1}{6}; b^T c^6 + 6\bar{b}^T c^5 = \frac{1}{7} \quad (3.4.11)$$

respectively. Solving the order conditions (3.4.10) and (3.4.11) we obtain a family of methods with four free parameters $c_1, c_2, c_3,$ and $c_4,$ provided $c_1 \neq c_2 \neq c_3 \neq c_4.$ Inserting $c = (0, 1, \frac{1}{2}, \frac{3}{4})^T$ we have the following tableau:

Tableau 4

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
$\frac{3}{4}$	$\frac{1431}{2048}$	$\frac{237}{4096}$	$\frac{-459}{4096}$	$\frac{27}{256}$	0	$\frac{27}{8192}$	$\frac{45}{8192}$	$\frac{-9}{512}$	0
		0	$\frac{251}{91}$	$\frac{-544}{91}$	$\frac{384}{91}$	$\frac{-46}{4095}$	$\frac{-523}{2730}$	$\frac{-1163}{1365}$	$\frac{-5648}{4095}$

3.5 A 5-stage, stage Order 9, 9th Order Generalised SDMIRK Method

We can represent a 5-stage, stage order 9, 9th order GSDMIRK method in the tableau below:

Tableau 5

0	0	0	0	0	0	0	0	0	0	0	0
1	1	0	0	0	0	0	0	0	0	0	0
c_3	v_3	x_{31}	x_{32}	x_{33}	x_{34}	0	\bar{x}_{31}	\bar{x}_{32}	\bar{x}_{33}	\bar{x}_{34}	0
c_4	v_4	x_{41}	x_{42}	x_{43}	x_{44}	0	\bar{x}_{41}	\bar{x}_{42}	\bar{x}_{43}	\bar{x}_{44}	0
c_5	v_5	x_{51}	x_{52}	x_{53}	x_{54}	0	\bar{x}_{51}	\bar{x}_{52}	\bar{x}_{53}	\bar{x}_{54}	0
		b_1	b_2	b_3	b_4	b_5	\bar{b}_1	\bar{b}_2	\bar{b}_3	\bar{b}_4	\bar{b}_5

Similarly setting $p = q = 9$ in (3.2.5) and (3.2.7) gives the order conditions of GSDMIRK in (3.1.1) and (3.1.2) as

$$\begin{aligned}
 Xe + v = c; \quad Xc + \bar{X}e + \frac{v}{2} = \frac{c^2}{2}; \quad \frac{Xc^2}{2} + \bar{X}c + \frac{v}{6} = \frac{c^3}{6}; \quad \frac{Xc^3}{6} + \frac{\bar{X}c^2}{2} + \frac{v}{24} = \frac{c^4}{24}; \quad \frac{Xc^4}{24} + \\
 \frac{\bar{X}c^3}{6} + \frac{v}{120} = \frac{c^5}{120}; \quad \frac{Xc^5}{120} + \frac{\bar{X}c^4}{24} + \frac{v}{720} = \frac{c^6}{720}; \quad \frac{Xc^6}{720} + \frac{\bar{X}c^5}{120} + \frac{v}{5040} = \frac{c^7}{5040}; \quad \frac{Xc^7}{5040} + \frac{\bar{X}c^6}{720} + \\
 \frac{v}{40320} = \frac{c^8}{40320}; \quad \frac{Xc^8}{40320} + \frac{\bar{X}c^7}{5040} + \frac{v}{362880} = \frac{c^9}{362880}
 \end{aligned} \tag{3.5.12}$$

and

$$\begin{aligned}
 b^T e = 1; \quad b^T c + b^T e = \frac{1}{2}; \quad b^T c^2 + 2\bar{b}^T c = \frac{1}{3}; \quad b^T c^3 + 3\bar{b}^T c^2 = \frac{1}{4}; \quad b^T c^4 + 4\bar{b}^T c^3 \\
 = \frac{1}{5}; \quad b^T c^5 + 5\bar{b}^T c^4 = \frac{1}{6}; \quad b^T c^6 + 6\bar{b}^T c^5 = \frac{1}{7}; \quad b^T c^7 + 7\bar{b}^T c^6 \\
 = \frac{1}{8}; \quad b^T c^8 + 8\bar{b}^T c^7 = \frac{1}{9}
 \end{aligned} \tag{3.5.13}$$

respectively. Solving the order conditions in (3.5.12) and (3.5.13) we obtain a family of methods with five free parameters c_1, c_2, c_3, c_4 and c_5 , provided $c_1 \neq c_2 \neq c_3 \neq c_4 \neq c_5$. Fixing $c = (0, 1, \frac{1}{3}, \frac{2}{3}, \frac{3}{4})^T$ we have the following tableau:

Tableau 6

0	0	0	0	0	0	0	0	0	0	0	0	0
1	1	0	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	0
$\frac{2}{3}$	$\frac{416}{729}$	$\frac{-49}{729}$	$\frac{38}{729}$	$\frac{1}{9}$	0	0	$\frac{5}{2187}$	$\frac{4}{2187}$	$\frac{-1}{81}$	$\frac{-2}{81}$	0	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	0
0	$\frac{35671}{287280}$	$\frac{5184}{16625}$	$\frac{55323}{10640}$	$\frac{-2080768}{448875}$	$\frac{1}{380}$		$\frac{61}{13680}$	$\frac{-297}{13300}$	$\frac{351}{2128}$	$\frac{512}{1995}$		

3.6 A 6-stage, stage order 11, 11th order Generalised SDMIRK Method

The tableau of a 6-stage, stage order 11, order 11 GSDMIRK method is considered as follows:

Tableau 7

1	1	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
c_3	v_3	x_{31}	x_{32}	x_{33}	x_{34}	x_{35}	0	\bar{x}_{31}	\bar{x}_{32}	\bar{x}_{33}	\bar{x}_{34}	\bar{x}_{35}	0	
c_4	v_4	x_{41}	x_{42}	x_{43}	x_{44}	x_{45}	0	\bar{x}_{41}	\bar{x}_{42}	\bar{x}_{43}	\bar{x}_{44}	\bar{x}_{45}	0	
c_5	v_5	x_{51}	x_{52}	x_{53}	x_{54}	x_{55}	0	\bar{x}_{51}	\bar{x}_{52}	\bar{x}_{53}	\bar{x}_{54}	\bar{x}_{55}	0	
c_6	v_6	x_{61}	x_{62}	x_{63}	x_{64}	x_{65}	0	\bar{x}_{61}	\bar{x}_{62}	\bar{x}_{63}	\bar{x}_{64}	\bar{x}_{65}	0	
		b_1	b_2	b_3	b_4	b_5	b_6	\bar{b}_1	\bar{b}_2	\bar{b}_3	\bar{b}_4	\bar{b}_5	\bar{b}_5	

Similarly setting $p = q = 11$ in (3.2.5) and (3.2.7) gives the order conditions of GSDMIRK in (3.1.1) and (3.1.2) as

$$\begin{aligned}
 Xe + v = c; \quad Xc + \bar{X}e + \frac{v}{2} = \frac{c^2}{2}; \quad \frac{Xc^2}{2} + \bar{X}c + \frac{v}{6} = \frac{c^3}{6}; \quad \frac{Xc^3}{6} + \frac{\bar{X}c^2}{2} + \frac{v}{24} = \frac{c^4}{24}; \quad \frac{Xc^4}{24} + \frac{\bar{X}c^3}{6} + \\
 \frac{v}{120} = \frac{c^5}{120}; \quad \frac{Xc^5}{120} + \frac{\bar{X}c^4}{24} + \frac{v}{720} = \frac{c^6}{720}; \quad \frac{Xc^6}{720} + \frac{\bar{X}c^5}{120} + \frac{v}{5040} = \frac{c^7}{5040}; \quad \frac{Xc^7}{5040} + \frac{\bar{X}c^6}{720} + \frac{v}{40320} = \\
 \frac{c^8}{40320}; \quad \frac{Xc^8}{40320} + \frac{\bar{X}c^7}{5040} + \frac{v}{362880} = \frac{c^9}{362880}; \quad \frac{Xc^9}{362880} + \frac{\bar{X}c^8}{40320} + \frac{v}{3628800} = \frac{c^{10}}{3628800}; \quad \frac{Xc^{10}}{3628800} + \\
 \frac{\bar{X}c^9}{362880} + \frac{v}{39916800} = \frac{c^{11}}{39916800}
 \end{aligned} \tag{3.6.14}$$

and

$$\begin{aligned}
b^T e &= 1; b^T c + b^T e = \frac{1}{2}; b^T c^2 + 2\bar{b}^T c = \frac{1}{3}; b^T c^3 + 3\bar{b}^T c^2 = \frac{1}{4}; b^T c^4 + 4\bar{b}^T c^3 \\
&= \frac{1}{5}; b^T c^5 + 5\bar{b}^T c^4 = \frac{1}{6}; b^T c^6 + 6\bar{b}^T c^5 = \frac{1}{7}; b^T c^7 + 7\bar{b}^T c^6 \\
&= \frac{1}{8}; b^T c^8 + 8\bar{b}^T c^7 = \frac{1}{9}; b^T c^9 + 9\bar{b}^T c^8 = \frac{1}{10}; b^T c^{10} + 10\bar{b}^T c^9 \\
&= \frac{1}{11}
\end{aligned} \tag{3.6.15}$$

respectively. Solving the order conditions in (3.6.14) and (3.6.15) we obtain a family of methods with six free parameters c_1, c_2, c_3, c_4, c_5 and c_6 , provided $c_1 \neq c_2 \neq c_3 \neq c_4 \neq c_5 \neq c_6$. Fixing $c = (0, 1, \frac{1}{2}, \frac{2}{3}, \frac{3}{4}, \frac{4}{3})^T$ we have the following tableau:

Tableau 8

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$\frac{1}{3}$	$\frac{184991}{2023391}$	$\frac{-220042}{3050865}$	$\frac{757079}{82373355}$	$\frac{-64412}{523125}$	$\frac{-3421}{4185}$	$\frac{4399824896}{10296669375}$	0	$\frac{4136}{3250865}$	$\frac{1439}{5491557}$	$\frac{-3314}{313875}$	$\frac{-79}{12555}$	$\frac{-31981568}{686444625}$	0	0
$\frac{2}{3}$	$\frac{195808}{203391}$	$\frac{-223757}{3050865}$	$\frac{323974}{82373355}$	$\frac{-1567}{523125}$	$\frac{-6236}{4185}$	$\frac{13040091136}{10296669375}$	0	$\frac{4811}{3050865}$	$\frac{640}{5491557}$	$\frac{-799}{313875}$	$\frac{-794}{12555}$	$\frac{-52953088}{686444625}$	0	0
$\frac{3}{4}$	$\frac{3912057}{40636232}$	$\frac{-47675871}{650117120}$	$\frac{2551701}{650117120}$	$\frac{-242159949}{81264640000}$	$\frac{-940827717}{650117120}$	$\frac{50637}{38750}$	0	$\frac{1024893}{650117120}$	$\frac{15123}{130023424}$	$\frac{-41275251}{16252928000}$	$\frac{40684761}{650117120}$	$\frac{-9633}{124000}$	0	0
$\frac{4}{3}$	$\frac{32783360}{203391}$	$\frac{-16782496}{3050865}$	$\frac{-1416929788}{82373355}$	$\frac{-73376}{523125}$	$\frac{-12685472}{4185}$	$\frac{-32113470472192}{10296669375}$	0	$\frac{8752288}{3050865}$	$\frac{-2856805}{5491557}$	$\frac{3048928}{313875}$	$\frac{1908848}{12555}$	$\frac{88852135936}{686444625}$	0	0
	0	$\frac{1172327}{10644480}$	$\frac{8328}{89375}$	$\frac{-493371}{80080}$	$\frac{40336031744}{57593913125}$	$\frac{7265463}{1757916160}$	$\frac{703}{80080}$	$\frac{79081}{23063040}$	$\frac{-102561}{2002000}$	$\frac{-267651}{640640}$	$\frac{-1122304}{6131125}$	$\frac{35313}{125565440}$		

In the next chapter, we shall investigate the stability properties of the GSDMIRK methods derived herein

CHAPTER FOUR

THE STABILITY OF THE GSDMIRK METHODS

4.1 Preamble

In this chapter, we determine the stability function as well as the region of absolute stability of each of our proposed methods in chapter three. Before the determination of the stability properties of the proposed GSDMIRK methods we shall consider the following definitions.

Definition 4.1

The region of absolute stability of GSDMIRK (3.1.1) is the set $l = \{z \in C: |w_j| < 1, j = 1, 2 \dots, k\}$. Fatunla (1978)

Definition 4.2

A GSDMIRK method is A-stable if the region of absolute stability includes in the entire left half of the z-plane (that is, $z \in (-\infty, 0)$). Fatunla (1978)

Definition 4.3

A GSDMIRK method is $A(\alpha)$ stable for some GSDMIRK $\alpha \in [0, \frac{\pi}{2})$ if the wedge $S_\alpha = \{z: |Arg(-z)| < \alpha, z \neq 0\}$ is contained in its region of absolute stability. Fatunla (1978)

4.2 Stability Function of GSDMIRK Methods

To determine the stability function of GSDMIRK, we write (3.1.2) as

$$Y_1 = (1 - v_1)y_n + v_1y_{n+1}$$

$$Y_2 = (1 - v_2)y_n + v_2y_{n+1} + hX_{21}F_1 + h^2\bar{X}_{21}\bar{F}_1$$

$$Y_3 = (1 - v_3)y_n + v_3y_{n+1} + h(X_{31}F_1 + X_{32}F_2) + h^2(\bar{X}_{31}\bar{F}_1 + \bar{X}_{32}\bar{F}_2)$$

$$\begin{array}{ccc} \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots \end{array}$$

$$Y_r = (1 - v_r)y_n + v_ry_{n+1} + h(X_{r1}F_1 \dots + X_{r,r-1}F_{r-1}) + h^2(\bar{X}_{r1}\bar{F}_1 \dots + \bar{X}_{r,r-1}\bar{F}_{r-1})$$

in vector form we have

$$Y = (1 - V)y_n + Vy_{n+1} + hXF + h^2\bar{X}\bar{F} \quad (4.2.1)$$

Applying the scalar test equation in (4.2.1), that is

$$\begin{cases} y' = f(x, y) = \lambda y \\ y'' = f'(x, y) = \lambda^2 y \end{cases} \quad (4.2.2)$$

we have

$$Y_r = (1 - V)y_n + Vy_{n+1} + hX(\lambda Y_r) + h^2\bar{X}(\lambda^2 Y_r) \quad (4.2.3)$$

putting $z = h\lambda$ in (4.2.3), we have

$$Y_r = (1 - V)y_n + Vy_{n+1} + zXY_r + z^2\bar{X}Y_r$$

$$Y_r - zXY_r - z^2\bar{X}Y_r = (1 - V)y_n + Vy_{n+1}$$

$$(1 - zX - z^2\bar{X})Y_r = (1 - V)y_n + Vy_{n+1}$$

$$Y_r = (1 - zX - z^2\bar{X})^{-1}[(1 - V)y_n + Vy_{n+1}] \quad (4.2.4)$$

similarly the output method (3.1.1) can be written as

$$y_{n+1} = y_n + hb^T F + h^2 \bar{b}^T \bar{F} \quad (4.2.5)$$

Applying (4.2.2) and putting $z = h\lambda$ in (4.2.5) yields

$$y_{n+1} = y_n + zb^T Y_r + z^2 \bar{b}^T Y_r \quad (4.2.6)$$

Putting (4.2.4) into (4.2.6) we have

$$y_{n+1} = y_n + zb^T (1 - zX - z^2 \bar{X})^{-1} [(1 - V)y_n + Vy_{n+1}] \\ + z^2 \bar{b}^T (1 - zX - z^2 \bar{X})^{-1} [(1 - V)y_n + Vy_{n+1}] \quad (4.2.7)$$

further simplification of (4.2.7) gives

$$y_{n+1} = \frac{[1 + zb^T (I - zX - z^2 \bar{X})^{-1} (e - v) + z^2 \bar{b}^T (I - zX - z^2 \bar{X})^{-1} (e - v)] y_n}{[1 + zb^T (I - zX - z^2 \bar{X})^{-1} (-v) + z^2 \bar{b}^T (I - zX - z^2 \bar{X})^{-1} (-v)]} \quad (4.2.8)$$

$$y_{n+1} = R(z) y_n \quad (4.2.9)$$

where $R(z)$ is the stability function, that is

$$R(z) = \frac{[1 + zb^T (I - zX - z^2 \bar{X})^{-1} (e - v) + z^2 \bar{b}^T (I - zX - z^2 \bar{X})^{-1} (e - v)]}{[1 + zb^T (I - zX - z^2 \bar{X})^{-1} (-v) + z^2 \bar{b}^T (I - zX - z^2 \bar{X})^{-1} (-v)]} \quad (4.2.10)$$

the compact form of (4.2.10) is

$$R(z) = \frac{\bar{P}(z, e - v)}{\bar{P}(z, -v)} \quad (4.2.11)$$

where;

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

The desired stability properties for a GSDMIRK scheme are given in terms of this stability function (4.2.10).

4.3 Stability Region of A 3-stage, Stage order 6, 6th Order GSDMIRK Method

Putting the values of ν , X , \bar{X} , b^T and \bar{b}^T in Tableau 2 into (4.2.10) gives the stability function of the order 6 GSDMIRK method as

$$R(z) = \frac{5760 - 3560z - 468z^2 + 462z^3 + 121z^4}{5760 - 9120z + 5772z^2 - 1710z^3 + 225z^4} \quad (4.3.12)$$

The boundary locus of the stability function (4.3.12) reveals that order 6 GSDMIRK method is A-stable, see Fig.1 for the stability plot.

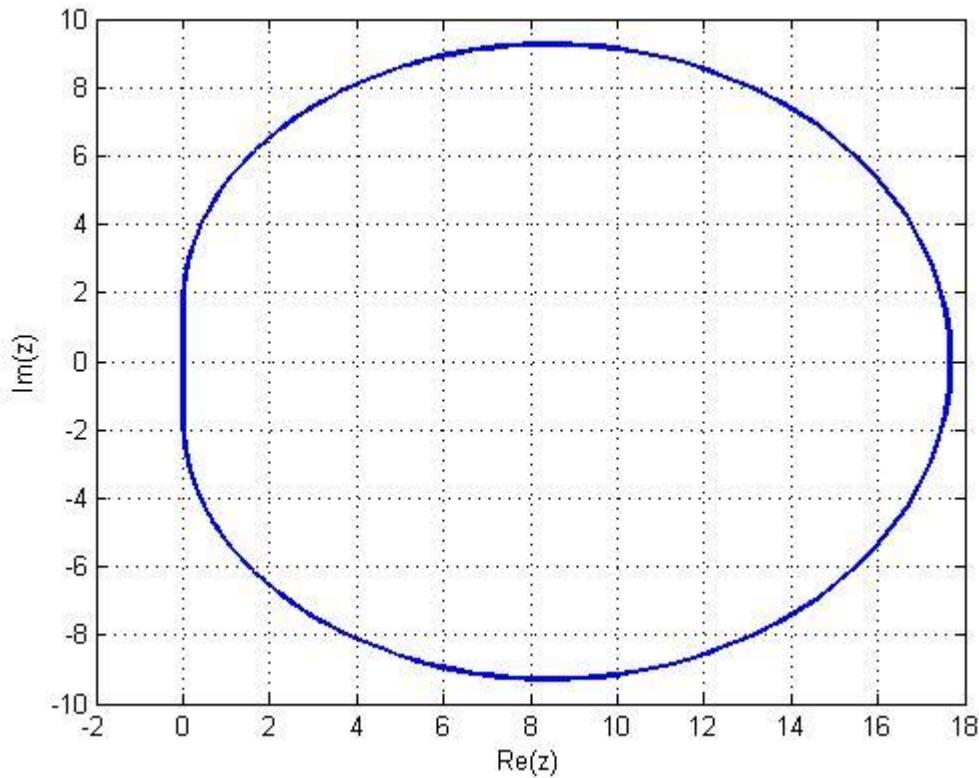


Fig. 1: The stability region of order 6 GSDMIRK method.

4.4 Stability Region of A 4-stage, Stage Order 7, 7th Order GSDMIRK Method

Inserting the values of v , X , \bar{X} , b^T and \bar{b}^T in Tableau 4 into (4.2.10), gives the stability function of the order 7 GSDMIRK method as

$$R(z) = \frac{16773120 - 28811520z - 15177120z^2 - 3221040z^3 - 381468z^4 - 27118z^5 - 1059z^6}{16773120 - 45584640z + 22020960z^2 - 5245200z^3 + 751812z^4 - 66906z^5 + 3177z^6} \quad (4.4.13)$$

The boundary locus of the stability function (4.4.13) shows that order 7 GSDMIRK method is A-stable, see Fig.2 for the stability plot.

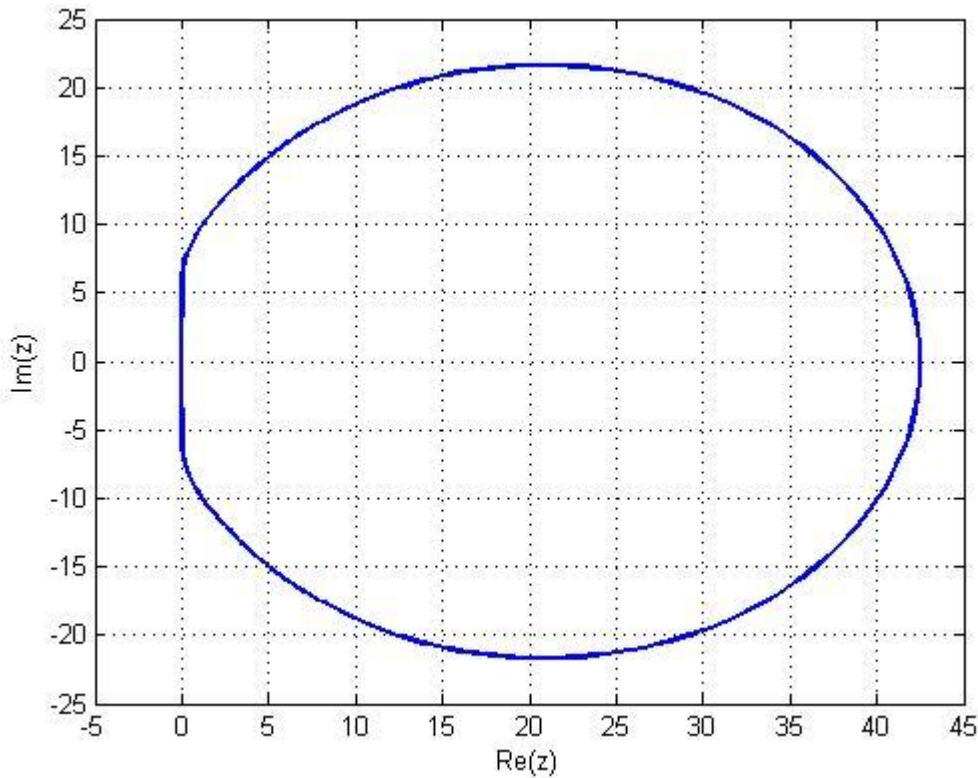


Fig. 2: The stability region of order 7 GSDMIRK method.

4.5 Stability Region of A 5-Stage, Stage Order 9, 9th Order GSDMIRK Method

Substituting the values v , X , \bar{X} , b^T and \bar{b}^T in Tableau 6 into (4.2.10) we obtain

$$R(z) = \frac{N(z)}{D(z)}, \tag{4.5.14}$$

where

$$N(z) = 1787114240 + 11378465280z + 3225594960z^2 + 54585900z^3 + 64691460z^4 + 4888512z^5 + 274095z^6 + 10441z^7 + 225z^8;$$

$$D(z) = 17871114240 + 6492648960z + 1423623600z^2 - 30977640z^3 + 39494220z^4 - 3704160z^5 + 344949z^6 - 20427z^7 + 675z^8.$$

The boundary locus curve of the stability function (4.5.14) shows that order 9 GSDMIRK method is $A(\alpha)$ -stable, $\alpha = 80^\circ$. See Fig.3 for the stability plot.

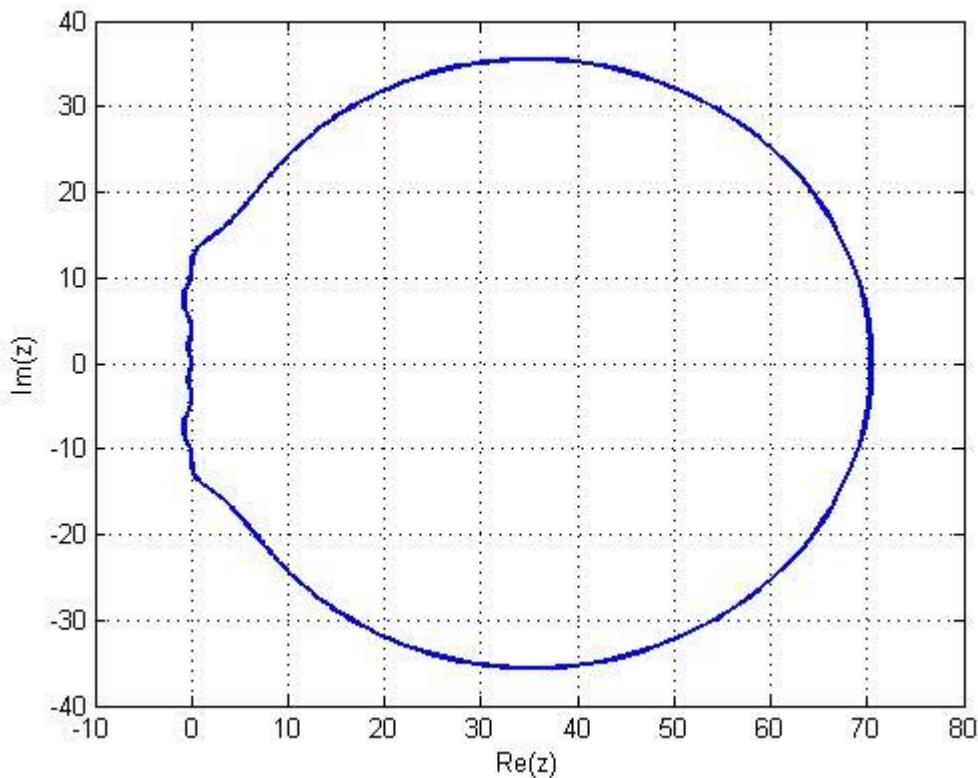


Fig. 3: The stability region of order 9 GSDMIRK method.

4.6 Stability Region of A 6-Stage, Stage Order 11, 11th Order SDMIRK Method

Putting the values of v , X , \bar{X} , b^T and \bar{b}^T as given in Tableau (8) into (4.2.10) we have the stability function for GSDMIRK method as;

$$R(z) = \frac{N(z)}{D(z)}, \quad (4.6.15)$$

where

$$N(z) = (-281448886118400 - 314202405888000z - 95083542550080z^2 - 14280918321600z^3 - 1212571571400z^4 - 51385155840z^5 + 573366600z^6 + 231709440z^7 + 16163478z^8 + 614829z^9 + 11771z^{10});$$

$$D(z) = 3(-93816295372800 - 10917839923200z + 26131473426240z^2 - 9796810343040z^3 + 2055535400520z^4 - 292791727080z^5 + 30487889700z^6 - 2387859812z^7 + 140019833z^8 - 5829114z^9 + 141252z^{10})$$

The boundary locus curve of the stability function (4.6.15) shows that order 11 GSDMIRK method is $A(\alpha)$ -stable, $\alpha = 84^0$. See Fig.4 for the stability plot.

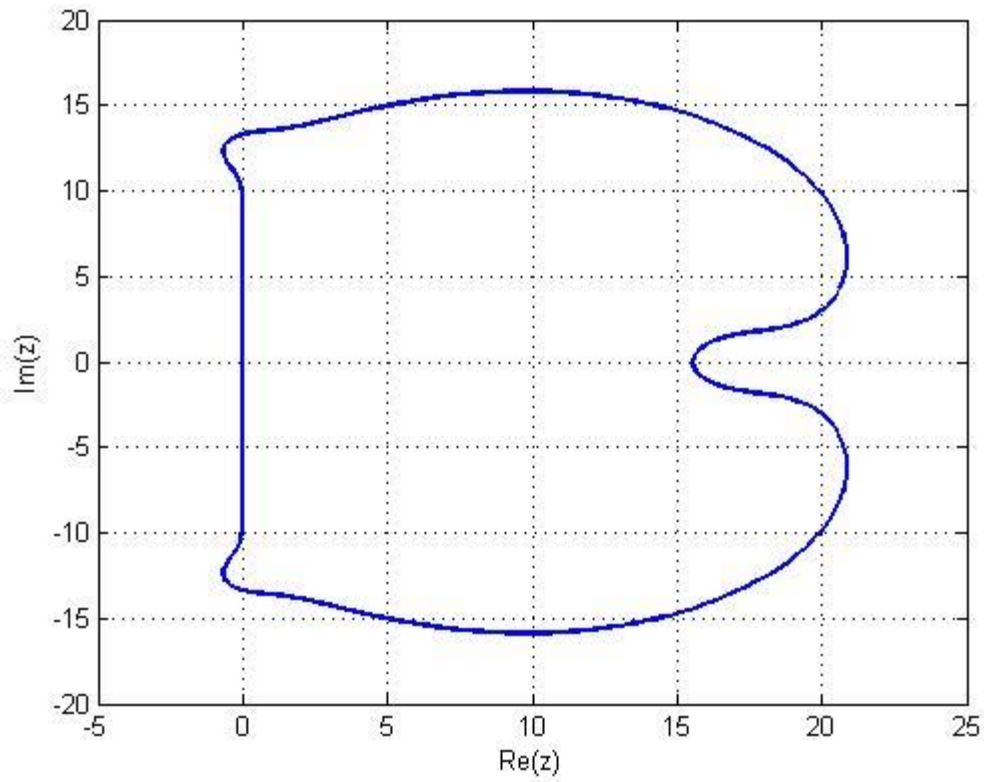


Fig. 4: The stability region of order 11 GSDMIRK method.

CHAPTER FIVE

IMPLEMENTATION AND CONCLUSION

5.1 Introduction

In this chapter, the conclusion of our work and implementation of the proposed GSDMIRK method in chapter three are considered. To illustrate how the methods are implemented we use the order six GSDMIRK method (see Tableau 2) to demonstrate the application of the methods and compared the results from our proposed methods with other existing methods (the order six second derivative backward difference formula (SDBDF), Hairer and Wanner (1996) and order six second derivative linear multi-step method (SDLMM), Enright (1974)) in the literature. The application of the SDMIRK method is in fixed step size approach. The non-linear equations defining the implicit stage values are

$$Y_r = (1 - v_r)y_n^{[j]} + v_r y_{n+1}^{[j]} + h \sum_{i=1}^{r-1} X_{ri} F(y_r^{[j]}) + h^2 \sum_{i=1}^s \bar{X}_{ri} \bar{F}(y_r^{[j]}), \quad (5.1.1)$$

are resolved by Newton – Raphson iterative method,

$$Y_r^{[j+1]} = Y_r^{[j]} - \left(I - hXJ(Y_r^{[j]}) - h^2 \bar{X}J'(Y_r^{[j]})^{-1} F(Y_r^{[j]}) \right), \quad (5.1.2)$$

where J and J' are the Jacobian matrices defined as

$$J(Y_r^{[j]}) = \varphi'(Y_r^{[j]}); J'(Y_r^{[j]}) = \varphi''(Y_r^{[j]}). \quad (5.1.3)$$

and I is the identity matrix.

Our starting values for (5.1.2) is obtained from the second derivative explicit Euler scheme, Onimanyi *et. al* (2012)

$$y_{n+1} = y_n + hf_n + \frac{h^2}{2} f'_n, \quad f' = \frac{\partial^2 f}{\partial x^2} = y''. \quad (5.1.4)$$

5.2 Numerical Results

We show the usefulness of our methods and also compare with exact solution by solving the following non-linear stiff problems:

Problem 1, Huang (2005):

$$y'_1 = -8y_1 + 7y_2, \quad y_1(0)=1, \quad y_1(x) = 2e^{-x} - e^{-50x}$$

$$y'_2 = 42y_1 - 43y_2, \quad y_2(0) = 8, \quad y_2(x) = 2e^{-x} + 6e^{-50x}$$

$$x \in [0,15]$$

This problem is mildly stiff, the eigen values are $\lambda_1 = -1$ and $\lambda_2 = -50$. The stiffness ratio is 50.

Problem 2, Abdi and Hojjati (2011)

$$y'_1 = -10004y_1 + y_2^4, \quad y_1(x) = e^{-4x} \quad y_1(0) = 1$$

$$y'_2 = y_1 - y_2(1 + y_2^3), \quad y_2(x) = e^{-x} \quad y_2(0) = 1,$$

$$x \in [0,15]$$

Problem 3, Ezzedine and Hojjati (2011)

$$y'_1 = -20y_1 - 0.25y_2 - 19.75y_3, \quad y_1(x) = \frac{1}{2}[e^{-0.5x} + e^{-20x}(\cos(20x) + \sin(20x))]$$

$$y'_2 = 20y_1 - 20.25y_2 - 20.25y_3, \quad y_2(x) = \frac{1}{2}[e^{-0.5x} - e^{-20x}(\cos(20x) + \sin(20x))],$$

$$y_3' = 20y_1 - 19.75y_2 - 0.25y_3, \quad y_3(x) = \frac{1}{2}[e^{-0.5x} + e^{-20x}(\cos(20x) + \sin(20x))]$$

$$x \in [0, 15], \quad y(0) = [1, 0, -1]^T$$

Problem 4, Prothero and Robinson (1974)

$$y'(x) = L(y - \phi(x) + \phi'(x)), y(0) = \phi(0)$$

$$y(x) = \phi(x), \quad \phi(x) = \sin(x), \quad L = 10^j, \quad j = 2(1)4$$

The following tables give the numerical results for the order six GSDMIRK (Tableau 2), order six SDBDF, Hairer and Wanner (1996) and order six SDLMM, Enright (1974) on the problems stated above using constant step size.

Table 1 Numerical results of problem 1 for fixed $h = 10^{-4}$

x	y_n	Error in GSDMIRK (Tableau 2)	Error in SDLMM Enright (1974)	Error in SDBDF Hairer and Wanner (1996)
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 2 Numerical results of problem 2 for fixed $h = 10^{-4}$

x	y_n	Error in GSDMIRK (Tableau 2)	Error in SDLMM Enright (1974)	Error in SDBDF Haire and Wanner (1996)
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 3 Numerical results of problem 3 for fixed $h = 10^{-4}$

x	y_n	Error in GSDMIRK (Tableau 2)	Error in SDLMM Enright (1974)	Error in SDBDF Hairer and Wanner (1996)
5.0	y_1	5.3114×10^{-7}	4.3170×10^{-6}	6.8191×10^{-6}
	y_2	1.0523×10^{-3}	4.0756×10^{-2}	3.5488×10^{-2}
	y_3	4.2842×10^{-7}	3.5537×10^{-6}	5.3987×10^{-6}
10.0	y_1	4.3598×10^{-8}	3.5436×10^{-7}	5.5975×10^{-7}
	y_2	8.6378×10^{-6}	3.3454×10^{-5}	2.9131×10^{-5}
	y_3	3.5167×10^{-8}	2.9171×10^{-7}	4.4315×10^{-7}
15.0	y_1	3.5788×10^{-9}	2.9171×10^{-7}	4.5947×10^{-8}
	y_2	7.0904×10^{-7}	2.7461×10^{-6}	2.3912×10^{-6}
	y_3	2.8866×10^{-9}	2.3945×10^{-8}	3.6376×10^{-8}

Table 4 Numerical results of problem 4 for fixed $h = 10^{-4}$

x	Error in GSDMIRK (Tableau 2)	Error in SDLMM Enright (1974)	Error in SDBDF Hairer and Wanner (1996)
0.2	4.2353×10^{-7}	5.7636×10^{-3}	1.8865×10^{-1}
0.4	3.8585×10^{-7}	0.11495×10^{-1}	3.7939×10^{-1}
0.6	3.3278×10^{-7}	1.6756×10^{-2}	5.5462×10^{-1}
0.8	2.6645×10^{-7}	2.133×10^{-2}	7.0733×10^{-1}
1.0	1.8949×10^{-7}	2.5056×10^{-2}	8.3144×10^{-1}

5.3 Discussion of Numerical Results

As earlier stated, the order six GSDMIRK (Tableau 2), order six SDLMM, Enright (1974) and order six SDBDF, Hairer and Wanner (1996) methods have been implemented on problems 1-4 and the results obtained are in tables 1-4 respectively. Fixed step size implementation was carried out and the absolute error obtained by finding the difference between the numerical solution $y_h(x)$ and the exact solution $y(x)$ for each of the problem is given in the tables 1-4.

Table 1 shows that the error obtain from the order six GSDMIRK method (Tableau 2) is far smaller than that obtained from the order six SDLMM, Enright (1974) and order six SDBDF,

Hairer and Wanner (1996) methods. Hence order six GSDMIRK method (Tableau 2) gives better accuracy.

Table 2 gives the absolute error obtained from the order six GSDMIRK method (Tableau 2), order six SDLMM, Enright (1974) and order six SDBDF, Hairer and Wanner (1996). The results in Table 2 confirm that the order six GSDMIRK method (Tableau 2) performs better than order six SDLMM, Enright (1974) and order six SDBDF, Hairer and Wanner (1996).

Table 3 shows that the error in order six GSDMIRK method (Tableau 2) is better than that of the order six SDLMM, Enright (1974) and order six SDBDF, Hairer and Wanner (1996).

Again Table 4 gives the absolute error obtained from the order six GSDMIRK method (Tableau 2), order six SDLMM, Enright (1974) and order six SDBDF, Hairer and Wanner (1996). The results in Table 4 reveal that the order six GSDMIRK method (Tableau 2) performs better than order six SDLMM, Enright (1974) and order six SDBDF, Hairer and Wanner (1996).

5.4 Summary

The development of numerical schemes for the numerical integration of IVPs (stiff and non-stiff) has been enhanced by the use of modern computing systems with higher processing speed.

This study comprises six chapters. In Chapter One, a brief introduction of the types of ODEs was discussed. In Chapter Two, RK methods were reviewed. In the same chapter, the MIRK methods were discussed and the general order conditions of the MIRK method were given. In chapter Three the derivation of the GSDMIRK methods were presented, while in Chapter Four, the stability properties of the proposed GSDMIRK methods were investigated. Chapter Five presents the numerical

implementation of our proposed method on stiff IVPs and also gives the summary and conclusion of the work. The study is concluded with references.

5.5 Conclusion

In this study, a class of generalized SDMIRK method has been introduced. This method is an extension (second derivative) of MIRK method discussed in Dow (2017). Investigation reveals that the new schemes enjoyed A -stable and $A(\infty)$ -stable stability properties. The order six GSDMIRK method (Tableau 2), order six SDLMM, Enright (1974) and order six SDBDF, Hairer and Wanner (1996) methods have been implemented on problems 1-4 and the results obtained reveal that the order six GSDMIRK method (Tableau 2) perform better than order six SDLMM, Enright (1974) and order six SDBDF, Hairer and Wanner (1996).

5.6 Future Investigation

Future research will investigate the derivation of L -stable members of GSDMIRK methods. Also further research can be made on how GSDMIRK methods can be casted as general linear methods (GLM).

5.7 Contribution to Knowledge

The study has contributed to knowledge in the following ways:

- a. construction of GSDMIRK methods for the integration of stiff ODEs
- b. derivation of A -stable and $A(\infty)$ -stable members of GSDMIRK methods
- c. derivation of GSDMIRK methods that attract easy and cheaper implementation cost.