IOSR Journal of Mathematics (IOSR-JM)
e-ISSN: 2278-5728, p-ISSN: 2319-765X. Volume 16, Issue 3 Ser. IV (May – June 2020), PP 39-46
www.iosrjournals.org

On The Derivation and Implementation of a Diagonally Implicit Runge Kutta Method for Solving Initial Value Problems in Ordinary Differential Equation

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Abstract: *In deriving a fifth order Runge-Kutta method, seventeen equations have to be satisfied. We made use of the row and column simplifying assumptions, together with the row-sum condition, to eliminate some of the occurring equations, thereby reducing the number of equations to be satisfied. The resulting method was implemented on some selected initial value problems and compare results with those of other method in the literature. The trajectory of the different errors associated with the results were investigated and drawn through the use of MATLAB package.*
Keywords: *Implicit method, Simplifying Assumptions, Stiff problem, Diagonally-implicit method.*

Date of Submission: 04-06-2020 Date of Acceptance: 20-06-2020

I. Introduction

Numerical methods of solution to ordinary differential equation problems have become indispensable due to their relevance in computational development. One such method is the Runge-Kutta method (RKM), which has been fully established as one good way of finding solutions to ODE problems. Hence Butcher (2003), asserts that Runge-Kutta methods (RKM) is a suitable way of obtaining numerical solutions to Ordinary Differential Equation (ODE), with various authors in the past deriving different methods to minimize the error associated little success. Ababneh, Ahmed and Ismail (2009), acknowledged that, the conventional numerical methods are in general, formulated on the basis of polynomial interpolation with the tacit assumption that Initial Value Problems (IVPs) satisfy the hypothesis of the existence and uniqueness theorem.

Numerical solutions for ODEs are very important in scientific computation, as they are widely used to proffer solutions to real-life world problems (Agbeboh, 2013). Problems in electrical circuits, chemical kinetics, vibrations, simple pendulum, rigid body rotation, atmospheric chemistry problems, biosciences and many more fields are modeled into ODEs as observed by Agbeboh, Aashikpelokhai and Aigbedion (2007).

However, ODE problems developed from these equations cannot be solved analytically, especially the case of nonlinear differential equations. Therefore they require the use of numerical methods to proffer accurate and stable solution to them. These problems arise in the form of non-stiff, singulo-stiff and stiff ordinary differential equations. Nevertheless, there are several ODEs, classified as Stiff equations, which some methods cannot handle very efficiently (Butcher & Jackiewicz (2003)). Some explicit methods cannot solve stiff ODE, hence the need for implicit methods.

The phenomenon of stiffness as Butcher (2016) puts it, was first recognized by Curtiss and Hirschfelder in 1952. Since then, an enormous amount of effort has gone into the analysis of stiff problems and, as a result, a great number of numerical methods have over the years been proposed for their solutions. Stiff problems have attracted the attention of many numerical analysts, which has led to the survey of methods for stiff problems developed by many authors (Lambert, 2000).

The importance of stiff equations is discussed by Butcher (2003), who present a comprehensive survey of application areas in which stiff equations arise. We emphasize that while the intuitive meaning of the term stiff is clear to all specialists, much controversy is going on about its mathematical definition. Implicit Runge-Kutta methods are more suitable than explicit methods for solving stiff problems because of their higher-order of accuracy

There are different types of Implicit Runge-Kutta Methods. These are the Singly Implicit Methods (SIRKM), Full Implicit Runge-Kutta Method (FIRKM) and the Diagonally Implicit Runge-Kutta Method (DIRKM). The construction of fully Implicit Methods are based on the theory of Gauss quadrature, where the nodes of integration are transformed zeros of Legendre polynomial from (-1,1) unto (0,1) as observed by Agam and Yahaya (2014). Also for methods of higher orders, their construction is very tedious because the zeros of

Legendre polynomial of order four and above are very complex, but the alternative methods to be used are those of Radau and Lobatto (Zlatev, 2016).

The construction of Diagonally Implicit Runge-Kutta Method is a recent development, since it reduces the computational time involved in implementing fully implicit methods. According to Butcher and Hojjati (2005), the diagonally implicit Runge-Kutta (DIRK) family of methods is possibly the most widely used implicit Runge-Kutta (IRK) methods in practical applications involving stiff, first-order, ordinary differential equations (ODEs) for initial value problems (IVPs) due to their relative ease of implementation,

Petzold (2013) showed that the degree of implicitness can be reduced by ensuring that the Runge-Kutta method has a lower triangular matrix. The idea here is to restrict the method to the form:

$$\begin{array}{c|ccccc} c_1 & \lambda \\ c_2 & a_{21} & \lambda \\ c_3 & a_{31} & a_{32} & \lambda \\ c_4 & \vdots & \vdots & \vdots & \ddots \\ c_5 & a_{s1} & a_{s2} & a_{s3} & a_{s4} & \lambda \\ \hline & b_1 & b_2 & b_3 & b_4 & b_s \end{array} . \quad (1.1)$$

where the diagonal entries λ are the same.

In this work, we will have a Diagonally Implicit Runge-Kutta method which has the form:

$$\begin{array}{c|ccccc} \lambda & \lambda \\ c_1 & a_{21} & \lambda \\ c_2 & a_{31} & a_{32} & \lambda \\ \vdots & \vdots & \vdots & \vdots & \ddots \\ c_s & b_1 & b_2 & b_3 & \dots & \lambda \\ \hline & b_1 & b_2 & b_3 & \dots & \lambda \end{array} . \quad (1.2)$$

where the last row of the matrix A, is the same with the weights"$b_i{}^s$"

We observed that the rooted tree approach of deriving the diagonally implicit Runge-Kutta method of order five, has seventeen equations to be satisfied. The equations associated with the order five method are given in Table 1 below.

TABLE 1

ORDER	EQUATION	NO.
1	$\sum_i b_i = 1$	T1
2	$\sum_i b_i c_i = \frac{1}{2}$	T2
3	$\sum_i b_i c_i^2 = \frac{1}{3}$	T3
3	$\sum_{ij} b_i a_{ij} c_j = \frac{1}{6}$	T4
4	$\sum_i b_i c_i^3 = \frac{1}{4}$	T5
4	$\sum_{ij} b_i c_i a_{ij} c_j = \frac{1}{8}$	T6
4	$\sum_{ij} b_i a_{ij} c_j^2 = \frac{1}{12}$	T7
4	$\sum_{ijk} b_i a_{ij} a_{jk} c_k = \frac{1}{24}$	T8
5	$\sum_i b_i c_i^4 = \frac{1}{5}$	T9

ORDER	EQUATION	NO.
5	$\sum_{ij} b_i c_i^2 a_{ij} c_j = \frac{1}{10}$	T10
5	$\sum_{ijk} b_i a_{ij} c_j a_{ik} c_k = \frac{1}{20}$	T11
5	$\sum_{ij} b_i c_i a_{ij} c_j^2 = \frac{1}{15}$	T12
5	$\sum_{ij} b_i a_{ij} c_j^3 = \frac{1}{20}$	T13
5	$\sum_{ijk} b_i c_i a_{ij} a_{jk} c_k = \frac{1}{30}$	T14
5	$\sum_{ijk} b_i a_{ij} c_j a_{jk} c_k = \frac{1}{40}$	T15
5	$\sum_{ijk} b_i a_{ij} a_{jk} c_k^2 = \frac{1}{60}$	T16
5	$\sum_{ijk} b_i a_{ij} a_{jk} a_{kl} c_l = \frac{1}{120}$	T17

II. Derivation Of Method

The general R-stage implicit Runge-Kutta method is defined by:

$$y_{n+1} - y_n = h\phi(x_n, y_n, h) \tag{2.1}$$

$$\phi(x_n, y_n, h) = \sum_{r}^{R} b_r k_r \tag{2.2}$$

$$k_r = f\left(x_n + hc_r,\; y_n + h\sum_{j=1}^{R} a_{rj} k_j \right) \qquad r = 1,2,3\ldots R \tag{2.3}$$

$$c_r = \sum_{r}^{R} a_{rj} \qquad r = 1,2,3\ldots R \tag{2.4}$$

Where the structure of (2.3) is, as in (1.2)

The derivation of implicit Runge-Kutta method, requires a procedure which is tedious and complicated. Therefore to reduce this process, we make use of two simplifying conditions for the columns and rows of the matrix of our method, given respectively as:

$$\sum_{i}^{s} b_i a_{ij} = (1 - c_j) \qquad j = 1,2,\ldots s \tag{2.5}$$

$$\sum_{j}^{s} a_{ij} c_j = \frac{1}{2} c_i^{\,2} \qquad i=1,2,\ldots s \tag{2.6}$$

And we also consider:

$$\sum_{i}^{s} b_i c_i^{\,k-1} = k^{-1} \qquad k= 1,2,\ldots s \tag{2.7}$$

From the seventeen equations above, the new method must satisfy equation (T1), (T2), (T3), (T5), and (T9). So by using MAPLE-18 package, we obtain the following parameters:

$$b_1 := 0;\ b_2 := \frac{8}{63} + \frac{1}{21}\sqrt{21};\ b_3 := \frac{125}{252};\ b_4 := \frac{8}{63} - \frac{1}{21}\sqrt{21};\ b_5 := \frac{1}{4};\ c_1 := \frac{1}{4};$$

$$c_2 := \frac{3}{5} - \frac{1}{10}\sqrt{21};\ c_3 := \frac{3}{5};\ c_4 := \frac{3}{5} + \frac{1}{10}\sqrt{21};\ c_5 := 1;$$

(2.8)

Next, using (2.5), equations (T4),(T7),(T8),(T13),(T15),(T16) and (T17) are eliminated from the set of equations because they are equivalent to some equations already satisfied above. And equation (2,6) is used to eliminate (T6),(T10) and (T11) for the same similar reason. In all, we are left with two equations, namely (T12) and (T14) which must be satisfied equally giving rise to the structure below.

$$\begin{array}{c|ccccc}
\frac{1}{4} & \frac{1}{4} & & & & \\
\frac{3}{5}-\frac{\sqrt{21}}{10} & \frac{7}{20}-\frac{\sqrt{21}}{10} & \frac{1}{4} & & & \\
\frac{3}{5} & a_{31} & a_{32} & \frac{1}{4} & & \\
\frac{3}{5}+\frac{\sqrt{21}}{10} & a_{41} & a_{42} & a_{43} & \frac{1}{4} & \\
1 & 0 & \frac{8}{63}+\frac{\sqrt{21}}{21} & \frac{125}{252} & \frac{8}{63}-\frac{\sqrt{21}}{21} & \frac{1}{4} \\
\hline
 & 0 & \frac{8}{63}+\frac{\sqrt{21}}{21} & \frac{125}{252} & \frac{8}{63}-\frac{\sqrt{21}}{21} & \frac{1}{4}
\end{array} \tag{2.9}$$

Using the row simplifying assumption and the row-sum condition, we have:

$$\sum_{j=1}^{5} a_{3,j} \cdot c_j = \frac{1}{2} \cdot c_3^2; \tag{2.10}$$

$$a_{32} := \frac{23}{100} + \frac{23}{350}\sqrt{21} \tag{2.11}$$

And consequently;

$$a_{3,1} := \frac{3}{25} - \frac{23}{350}\sqrt{21} \tag{2.12}$$

to get a new structure:

$$\begin{array}{c|cccccc}
\frac{1}{4} & \frac{1}{4} & & & & & \\
\frac{3}{5}-\frac{\sqrt{21}}{10} & \frac{7}{20}-\frac{\sqrt{21}}{10} & \frac{1}{4} & & & & \\
\frac{3}{5} & \frac{3}{25}-\frac{23\sqrt{21}}{350} & \frac{23}{100}+\frac{23\sqrt{21}}{350} & \frac{1}{4} & & & \\
\frac{3}{5}+\frac{\sqrt{21}}{10} & a_{41} & a_{42} & a_{43} & \frac{1}{4} & & \\
1 & 0 & \frac{8}{63}+\frac{\sqrt{21}}{21} & \frac{125}{252} & \frac{8}{63}-\frac{\sqrt{21}}{21} & \frac{1}{4} \\
\hline
 & 0 & \frac{8}{63}+\frac{\sqrt{21}}{21} & \frac{125}{252} & \frac{8}{63}-\frac{\sqrt{21}}{21} & \frac{1}{4}
\end{array} \tag{2.13}$$

In order to determine the remaining variables, i.e., a_{42} and a_{43}, we make use of equation (T12) and (T14):
Equation (T12) is given as:

$$\sum_{i=1}^{5}\sum_{j=1}^{5} b_i \cdot c_i \cdot a_{i,j} \cdot c_j^2 = \frac{1}{15}; \tag{2.14}$$

Expanding and simplifying (2.14), we obtain:

$$a_{4,2} = -\frac{1}{28}\,\frac{-1035\sqrt{21} + 9660 + 3808\sqrt{21}\,a_{4,3} - 29988\,a_{4,3}}{664\sqrt{21} - 2979} \tag{2.15}$$

while that of (T14) is given as:

$$\sum_{i=1}^{5}\sum_{j=1}^{5}\sum_{k=1}^{5} b_i \cdot c_i \cdot a_{i,j} \cdot a_{j,k} \cdot c_k = \frac{1}{30}; \tag{2.16}$$

Expanding and simplifying (2.16), substituting into (2.15), we obtain:

$$a_{43} := \frac{8153897}{45515220}\sqrt{21} - \frac{9196397}{30343480} \quad \text{and} \quad a_{42} := \frac{20860472}{398258175}\sqrt{21} + \frac{97356541}{151717400}$$

and using the row-sum condition,

$$a_{41} := \frac{863267}{75858700} - \frac{69841671}{531010900}\sqrt{21}$$

which makes the method to be given as:

$$y_{n+1} = y_n + h\left(\left(\frac{8}{63}+\frac{\sqrt{21}}{21}\right)k_2 + \frac{125}{252}k_3 + \left(\frac{8}{63}+\frac{\sqrt{21}}{21}\right)k_4 + \frac{1}{4}k_5\right) \tag{2.17}$$

with the slopes as:

$$k_1 = f\left(x_1 + \frac{1}{4}h,\quad y_1 + h\left(\frac{1}{4}k_1\right)\right)$$

$$k_2 = f\left(x_1 + \left(\frac{3}{5} - \frac{\sqrt{21}}{10}\right)h,\quad y_1 + h\left(\left(\frac{7}{20} - \frac{\sqrt{21}}{10}\right)k_1 + \frac{1}{4}k_2\right)\right)$$

$$k_3 = f\left(x_1 + \left(\frac{3}{5}\right)h,\quad y_1 + h\left(\left(\frac{3}{25} - \frac{23\sqrt{21}}{350}\right)k_1 + \left(\frac{23}{100} + \frac{23\sqrt{21}}{350}\right)k_2 + \frac{1}{4}k_3\right)\right)$$

$$k_4 = f\left(x_1 + \left(\frac{3}{5} + \frac{\sqrt{21}}{10}\right)h,\quad y_1 + h\left(\left(\frac{863267}{75858700} - \frac{69841671\sqrt{21}}{531010900}\right)k_1 + \left(\frac{20860472\sqrt{21}}{398258175} + \frac{97356541}{151717400}\right)k_2 + \left(\frac{8153897\sqrt{21}}{45515220} + \frac{9196397}{30343480}\right)k_3 + \frac{1}{4}k_4\right)\right)$$

$$k_5 = f\left(x_1 + h,\quad y_1 + h\left(\left(\frac{8}{63} + \frac{\sqrt{21}}{21}\right)k_2 + \frac{125}{252}k_3 + \left(\frac{8}{63} - \frac{\sqrt{21}}{21}\right)k_4 + \frac{1}{4}k_5\right)\right)$$

(2.18)

III. Implementation Of Method:

In order to ascertain the suitability of our method, we selected some stiff initial value problems whose solution were provided by our method and compared with other existing implicit method, of the same order as given below:.

Problem 1. $y' = -1000y(x) + e^{-2x}; y(0) = 0$ (Ababneh, Ahmed and Ismail (2009))

Theoretical solution $\frac{1}{998}e^{-2x} - \frac{1}{998}e^{-1000x}$

Problem 2. $y' = -200(y(x) - \cos(x));\ y(0) = 0$; (Ababneh, Ahmed and Ismail (2009))

Theoretical solution $\frac{40000}{40001}\cos(x) + \frac{200}{40001}\sin(x) - \frac{40000}{40001}e^{-200x}$

Problem 3. $y' = -8y + 8x + 1;\ y(0) = 2$; (Ababneh, Ahmed and Ismail (2009))

Theoretical solution $x + 2\cdot e^{(-8\cdot x)}$

Problem 4. $y' = x^3 + y, \quad y(0) = 2$ (Butcher, J.C. (2016))

Theoretical solution $-x^3 - 3x^2 - 6x - 6 + 8x^x$

TABLE 2

		$y' = -1000y + e^{(-2x)},\ y(0) = 0,\ h = 0.001$			
		NEW METHOD		DIRKM(5,5)	
XN	TSOL	YN	ERROR	YN	ERROR
0.001	0.00063138533	0.00063148580	1.00473903E-07	0.00063360667	2.22133853E-06
0.002	0.00086239750	0.00086247141	7.39113573E-08	0.00086402694	1.62943542E-06
0.003	0.00094612314	0.00094616392	4.07764403E-08	0.00094701958	8.96435818E-07
0.004	0.00097566761	0.00097568761	1.99943295E-08	0.00097610598	4.38372505E-07
0.005	0.00098528245	0.00098529164	9.18889822E-09	0.00098548342	2.00966765E-07
0.006	0.00098756810	0.00098757215	4.05158210E-09	0.00098765654	8.84382626E-08
0.007	0.00098715998	0.00098716172	1.73423500E-09	0.00098719781	3.78296571E-08
0.008	0.00098576338	0.00098576411	7.24535486E-10	0.00098577923	1.58434434E-08
0.009	0.00098400563	0.00098400593	2.95280874E-10	0.00098401216	6.52350767E-09
0.01	0.00098211750	0.00098211762	1.16112923E-10	0.00098212015	2.64454207E-09

TABLE 3

		$y' = -200\left(y - \cos(x)\right),\ y(0)=0,\ h=0.001$			
		NEW METHOD		DIRKM(5,5)	
XN	TSOL	YN	ERROR	YN	EEROR
0.001	0.18126921519	0.18127119635	1.98115487E-06	0.18129286829	2.36531023E-05
0.002	0.32967971197	0.32968295605	3.24408035E-06	0.32971844257	3.87306066E-05
0.003	0.45118758420	0.45119156826	3.98406509E-06	0.45123514859	4.75643923E-05
0.004	0.55066926911	0.55067361831	4.34919795E-06	0.55072119181	5.19227060E-05
0.005	0.63211725582	0.63212170688	4.45106280E-06	0.63217039370	5.31378813E-05
0.006	0.69880031795	0.69880469106	4.37310711E-06	0.69885252423	5.22062746E-05
0.007	0.75339470101	0.75339887818	4.17717592E-06	0.75344456730	4.98662938E-05
0.008	0.79809152946	0.79809543806	3.90860167E-06	0.79813818864	4.66591772E-05
0.009	0.83468474433	0.83468834448	3.60015848E-06	0.83472772054	4.29762139E-05
0.01	0.86464310027	0.86464637540	3.27512553E-06	0.86468219559	3.90953227E-05

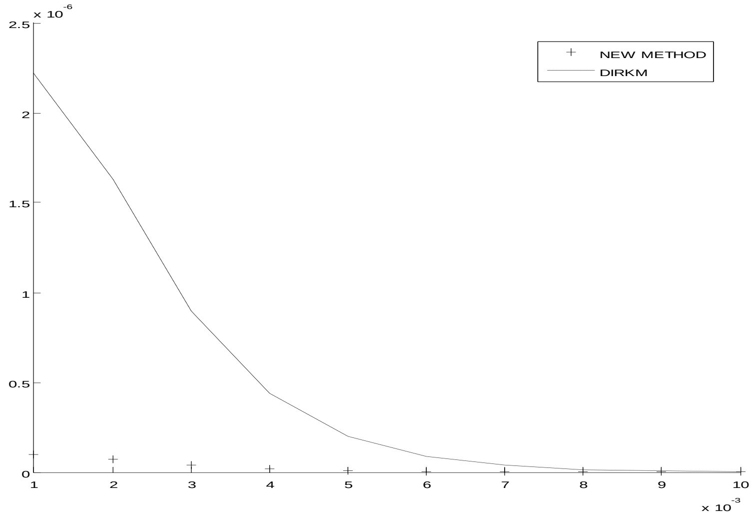
TABLE 4

		$y' = -8y + 8x + 1,\ y(0)=2,\ h=0.01$			
		NEW METHOD		DIRKM(5,5)	
XN	TSOL	YN	ERROR	YN	ERROR
0.01	1.85623269277	1.85623250712	1.85657344E-07	1.85622971810	2.97467746E-06
0.02	1.72428757793	1.72428723517	3.42766642E-07	1.72428208599	5.49194235E-06
0.03	1.60325572213	1.60325524751	4.74620211E-07	1.60324811759	7.60454651E-06
0.04	1.49229807415	1.49229748998	5.84172871E-07	1.49228871431	9.35983405E-06
0.05	1.39064009207	1.39063941800	6.74074374E-07	1.39062929181	1.08002611E-05
0.06	1.29756678361	1.29756603691	7.46698850E-07	1.29755481975	1.19638674E-05
0.07	1.21241812770	1.21241732353	8.04171526E-07	1.21240524299	1.28847048E-05
0.08	1.13458484809	1.13458399969	8.48392964E-07	1.13457125486	1.35932252E-05
0.09	1.06350451192	1.06350363086	8.81061046E-07	1.06349039529	1.41166330E-05
0.1	0.99865792823	0.99865702454	9.03690903E-07	0.99864344903	1.44792047E-05

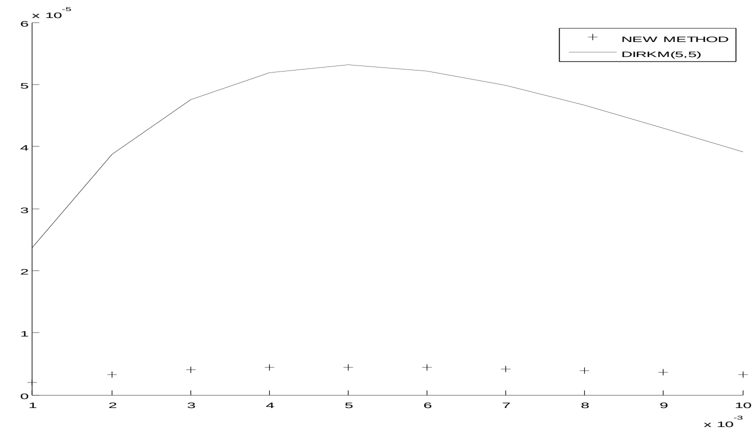
TABLE 5

		$y' = x^3 + y,\quad y(0)=2,\quad h=0.1$			
		NEW METHOD		DIRKM(5,5)	
XN	TSOL	YN	ERROR	YN	ERROR
0.1	2.2103673446	2.2103673113	3.3320768E-08	2.210372586	5.2409665E-06
0.2	2.4432220653	2.4432220763	1.0981676E-08	2.443233849	1.1783651E-05
0.3	2.7018704606	2.7018705995	1.3891255E-07	2.701890458	1.9996970E-05
0.4	2.9905975811	2.9905979380	3.5688166E-07	2.990627894	3.0313039E-05
0.5	3.3147701656	3.3147708373	6.7172203E-07	3.314813402	4.3236388E-05
0.6	3.6809504031	3.6809514938	1.0907081E-06	3.681009758	5.9354415E-05
0.7	4.0970216598	4.0970232813	1.6215728E-06	4.097101009	7.9349231E-05
0.8	4.5723274279	4.5723297005	2.2725238E-06	4.572431439	1.0401109E-04
0.9	5.1178248893	5.1178279415	3.0522578E-06	5.117959143	1.3425359E-04
1	5.7462546277	5.7462585976	3.9699723E-06	5.746425759	1.7113088E-04

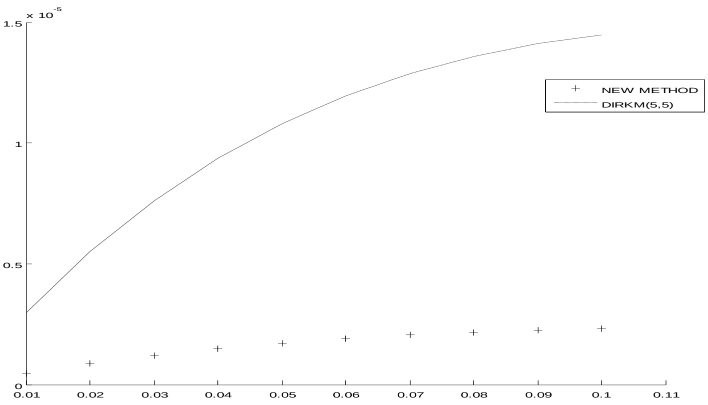
IV. Error Analysis



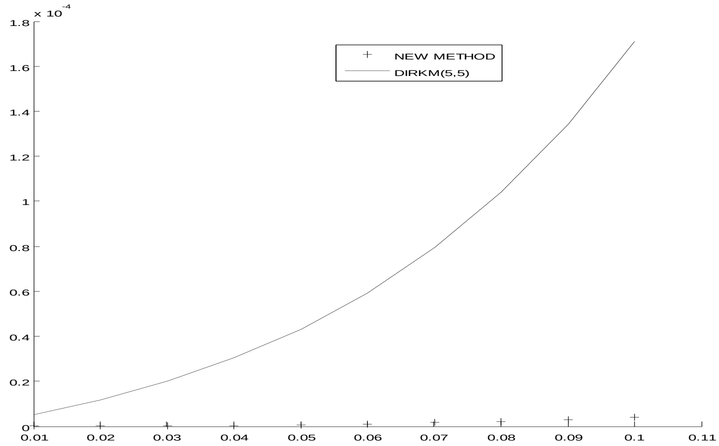
ERROR ANALYSIS FOR PROBLEM 1



ERROR ANALYSIS FOR PROBLEM 2



ERROR ANALYSIS FOR PROBLEM 3



ERROR ANALYSIS FOR PROBLEM 4

V. Discussion

The research conducted in this paper shows the possibility of constructing new diagonally implicit Runge-Kutta five-stage fifth order formula with L-stability property. We apply the new DIRKM to the above IVPs and the results generated by the method in this paper evidently proved the extent of accuracy of the method in comparison with the other method of the same order. That is, the newly derived method is more accurate as seen from the computational results presented in Tables 2,3,4 and 5, since its absolute errors are the least upon implementation on the initial value problems presented in this paper. It therefore follows that the new scheme is quite efficient, and conclude that the method proposed is reliable, stable and with high accuracy in computation.

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IOSR Journal of Mathematics (IOSR-JM), 16(3), (2020): pp. 39-46.