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A Class of Rational Integrator Scheme of Order 10: Derivation and Implementation

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ABSTRACT: *In this research, we derive a rational integrator method of order 10 for the solution of Ordinary Differential Equations (ODES), in line with the general representation given by Aashikpelokhai (1991). This was achieved by considering the Rational Interpolation Formula* $y_{n+1}=\left(\sum_{r=0}^{L} p_r x_{n+1}^r\right)\left(1+\sum_{r=1}^{M} q_r x_{n+1}^r\right)^{-1}$ *where L and M are the degrees of the respective numerator and denominator polynomials. There are three mutually exclusive forms the above integrator can assume one at a time. The forms are when L < M, L = M and L > M ; This work concentrates on deriving a method when L > M, and on expansion and comparing with the corresponding Taylor series, the resulting expression was used to determine the interpolation parameters* p_r, q_r *using Crammer's method, which was simplified to get a new method of order 10. The new method was used to solve some selected stiff initial value problems and the result therein, compared favorably well with those of other existing schemes.*

Keywords: *Interpolation, Stiff-problem, Initial value and Taylor-Series.*

I. INTRODUCTION

Numerical methods for systems of Ordinary Differential Equations (ODEs) have been attracting much attention due to their need in the solution of problems arising from the mathematical formulation of physical situations in chemical kinetics, population models, mechanical oscillations, planetary motions, electrical networks, nuclear reactor control, tunnel switching problems, which often lead to Initial Value Problems (IVPs) in Ordinary Differential Equations that are stiff, singular or oscillatory. Our computational experience as exemplified by the works in Aashikpelokhai (1991, 2000), Fatunla and Aashikpelokhai (1994), Elakhe and Aashikpelokhai (2013) along with the research work given by Fatunla (1982), Lambert and Shaw (1965), Otunta and Ikhile (1996, 1999), all give credence to the need for rational integrators. There are quite a number of initial value problems that are stiff; they are mainly from Reaction, Chemical kinetic and Life Sciences, Aashikpelokhai (1996,2000), Momodu (2006), Nunn and Huang (2005), Lambert (1973,2000), Corless (2001), Abhulimen and Otunta, (2007),Vigo and Martin (2006). The problem for this research paper is to derive a new method and proffer numerical solutions to some of these ODE problems, which are in the form of initial value problems, which are represented by:

$$f\left(x,y\right),\ \ y\left(x_0\right)=y_0,\ \ a\le x\le b \tag{1}$$

whose solution function $y' \in [a,b \to R]$, where a and b are finite.

II. DERIVATION OF METHOD

Our derivation of the rational interpolation method consists of matching the Taylor series expansion of $y(x_{n+1})$ with the approximation value of y_{n+1}. At the point $x = x_n$ in the interval $[x_n, x_{n+1}]$ we set $y_n = y(x_n)$, since Our Taylor series about x_n for both $y(x_{n+1})$ and y_{n+1} require the use of $h = x_{n+1} - x_n$, we choose h sufficiently small enough so that x_{n+1} and x_n are very close. In the derivation of our method we will analyze the case when $L > M$ and so the general rational interpolation method is defined as:

$$U(x) = \frac{\sum_{r=0}^{7} p_r x^r}{1 + \sum_{r=1}^{3} q_r x^r} \qquad (2)$$

where $p_0, p_1, p_2 ... p_r$ and q_1, q_2, q_3 are integrator parameters to be determined. But

$$U(x) = \sum_{r=0}^{\infty} c_r x^r \qquad (3)$$

Hence (2) can be written as:

$$\sum_{r=0}^{\infty} c_r x^r = \frac{\sum_{r=0}^{7} p_r x^r}{1 + \sum_{r=1}^{3} q_r x^r} \qquad (4)$$

$$\sum_{r=0}^{\infty} c_r x^r \left(1 + \sum_{r=1}^{3} q_r x^r\right) = \sum_{r=0}^{7} p_r x^r \qquad (5)$$

On expanding (5), we get

$$\begin{bmatrix} (c_7 q_3 + c_8 q_2 + c_9 q_1 + c_{10}) x^{10} + (c_6 q_3 + c_7 q_2 + c_8 q_1 + c_9) x^9 \\ +(c_5 q_3 + c_6 q_2 + c_7 q_1 + c_8) x^8 + (c_4 q_3 + c_5 q_2 + c_6 q_1 + c_7) x^7 \\ +(c_3 q_3 + c_4 q_2 + c_5 q_1 + c_6) x^6 + (c_2 q_3 + c_3 q_2 + c_4 q_1 + c_5) x^5 \\ +(c_1 q_3 + c_2 q_2 + c_3 q_1 + c_4) x^4 + (c_0 q_3 + c_1 q_2 + c_2 q_1 + c_3) x^3 \\ +(c_0 q_2 + c_1 q_1 + c_2) x^2 + (c_0 q_1 + c_1) x \\ = x^7 p_7 + x^6 p_6 + x^5 p_5 + x^4 p_4 + x^3 p_3 + x^2 p_2 + x p_1 + p_0 \end{bmatrix} \qquad (6)$$

We compare the coefficients of x, and get the following equations:

$$\begin{aligned} p_0 &= c_0 \\ p_1 &= (c_0 q_1 + c_1) \\ p_2 &= (c_0 q_2 + c_1 q_1 + c_2) \\ p_3 &= (c_0 q_3 + c_1 q_2 + c_2 q_1 + c_3) \\ p_4 &= (c_1 q_3 + c_2 q_2 + c_3 q_1 + c_4) \\ p_5 &= (c_2 q_3 + c_3 q_2 + c_4 q_1 + c_5) \end{aligned} \qquad \textbf{(7)}$$

$$p_6 = (c_3 q_3 + c_4 q_2 + c_5 q_1 + c_6)$$
$$p_7 = (c_4 q_3 + c_5 q_2 + c_6 q_1 + c_7)$$
$$p_8 = (c_5 q_3 + c_6 q_2 + c_7 q_1 + c_8)$$
$$p_9 = (c_6 q_3 + c_7 q_2 + c_8 q_1 + c_9) \quad (8)$$
$$p_{10} = (c_7 q_3 + c_8 q_2 + c_9 q_1 + c_{10})$$

Since $p_8, p_9, p_{10}\ldots$ are equivalent to zero, then

$$(c_5 q_3 + c_6 q_2 + c_7 q_1 + c_8) = 0$$
$$(c_6 q_3 + c_7 q_2 + c_8 q_1 + c_9) = 0 \quad (9)$$
$$(c_7 q_3 + c_8 q_2 + c_9 q_1 + c_{10}) = 0$$

This can be written as

$$(c_5 q_3 + c_6 q_2 + c_7 q_1 + c_8) = -c_8$$
$$(c_6 q_3 + c_7 q_2 + c_8 q_1 + c_9) = -c_9 \quad (10)$$
$$(c_7 q_3 + c_8 q_2 + c_9 q_1 + c_{10}) = -c_{10}$$

Rearranging and putting (10) in matrix form, gives:

$$\begin{bmatrix} c_9 & c_8 & c_7 \\ c_8 & c_7 & c_6 \\ c_7 & c_6 & c_5 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} = \begin{bmatrix} -c_{10} \\ -c_9 \\ -c_8 \end{bmatrix} \quad (11)$$

The above equation which can be put in the form:

$$Aq = b \quad (12)$$

Where

$$A = \begin{bmatrix} c_9 & c_8 & c_7 \\ c_8 & c_7 & c_6 \\ c_7 & c_6 & c_5 \end{bmatrix} \quad (13)$$

$$q = \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} \quad (14)$$

and

$$b = \begin{bmatrix} -c_{10} \\ -c_9 \\ -c_8 \end{bmatrix} \quad (15)$$

The governing equation (11) will be used to derive the new method.

Now, to solve for $q_i^s,\ i=1,2,3,$ we use the crammer's rule which is given as

$$q_i = \frac{x_i}{|A|} \tag{16}$$

First, we construct the determinants from (11) as follows:

$$A = \begin{bmatrix} c_9 & c_8 & c_7 \\ c_8 & c_7 & c_6 \\ c_7 & c_6 & c_5 \end{bmatrix} \tag{17}$$

$$x_1 = \begin{bmatrix} -c_{10} & c_8 & c_7 \\ -c_9 & c_7 & c_6 \\ -c_8 & c_6 & c_5 \end{bmatrix} \tag{18}$$

$$x_2 = \begin{bmatrix} c_9 & -c_{10} & c_7 \\ c_8 & -c_9 & c_6 \\ c_7 & -c_8 & c_5 \end{bmatrix} \tag{19}$$

$$x_3 = \begin{bmatrix} c_9 & c_8 & -c_{10} \\ c_8 & c_7 & -c_9 \\ c_7 & c_6 & -c_8 \end{bmatrix} \tag{20}$$

$$q_1 = \frac{\left(-c_{10}c_5c_7 + c_{10}c_6^2 + c_5c_8c_9 - c_6c_7c_9 - c_6c_8^2 + c_7^2c_8\right)}{\left(c_5c_7c_9 - c_5c_8^2 - c_6^2c_9 + 2c_6c_7c_8 - c_7^3\right)} \tag{21}$$

$$q_2 = \frac{\left(c_{10}c_5c_8 - c_{10}c_6c_7 - c_5c_9c_9 + c_6c_9c_8 + c_7^2c_9 - c_7c_8c_8\right)}{\left(c_5c_7c_9 - c_5c_8^2 - c_6^2c_9 + 2c_6c_7c_8 - c_7^3\right)} \tag{22}$$

$$q_3 = \frac{\left(-c_{10}c_6c_8 + c_{10}c_7^2 + c_6c_9c_9 - c_7c_8c_9 - c_7c_9c_8 + c_8^2c_8\right)}{\left(c_5c_7c_9 - c_5c_8^2 - c_6^2c_9 + 2c_6c_7c_8 - c_7^3\right)} \tag{23}$$

At this point, taking $x = x_{n+1}$, (3) becomes:

$$y_{n+1} = \sum_{r=0}^{\infty} c_r x_{n+1}^r \tag{24}$$

So by Taylor series expansion of y_{n+1} we have:

$$y_{n+1} = \sum_{r=0}^{\infty} \frac{h^r y_n^{(r)}}{r!} \tag{25}$$

Therefore:

$$\sum_{r=0}^{\infty} c_r x_{n+1}^r = \sum_{r=0}^{\infty} \frac{h^r y_n^{(r)}}{r!} \tag{26}$$

Expanding (26)(Taylor series), and comparing coefficients, we have:

$$\begin{aligned}
&c_0 = y_n, c_1 = \frac{h y_n^{(1)}}{1! x_{n+1}^1}, c_2 = \frac{h^2 y_n^{(2)}}{2! x_{n+1}^2}, c_3 = \frac{h^3 y_n^{(3)}}{3! x_{n+1}^3},\\
&c_4 = \frac{h^4 y_n^{(4)}}{4! x_{n+1}^4}, c_5 = \frac{h^5 y_n^{(5)}}{5! x_{n+1}^5}, c_6 = \frac{h^6 y_n^{(6)}}{6! x_{n+1}^6}\\
&c_7 = \frac{h^7 y_n^{(7)}}{7! x_{n+1}^7}, c_8 = \frac{h^8 y_n^{(8)}}{8! x_{n+1}^8}, c_9 = \frac{h^9 y_n^{(9)}}{9! x_{n+1}^9},\\
&c_{10} = \frac{h^{10} y_n^{(10)}}{10! x_{n+1}^{10}}
\end{aligned} \tag{27}$$

From (16), with some simplifications, we obtain expressions for the following:

$$q_1 x_{n+1} = \frac{-h\begin{pmatrix}168 y^{(5)} y^{(7)} y^{(10)} - 196 y^{(6)^2} y^{(10)} - 210 y^{(5)} y^{(8)} y^{(9)} \\ -360 y^{(7)^2} y^{(8)} + 280 y^{(6)} y^{(7)} y^{(9)} + 315 y^{(6)} y^{(8)^2}\end{pmatrix}}{10\begin{pmatrix}168 y^{(5)} y^{(7)} y^{(9)} - 189 y^{(5)} y^{(8)^2} - 288 y^{(7)^3} \\ +504 y^{(6)} y^{(7)} y^{(8)} - 196 y^{(6)^2} y^{(9)}\end{pmatrix}}$$

$$q_2 x_{n+1}^2 = \frac{h^2\begin{pmatrix}63 y^{(5)} y^{(8)} y^{(10)} - 84 y^{(6)} y^{(7)} y^{(10)} - 70 y^{(5)} y^{(9)^2} \\ +120 y^{(7)^2} y^{(9)} - 135 y^{(7)} y^{(8)^2} + 105 y^{(6)} y^{(8)} y^{(9)}\end{pmatrix}}{30\begin{pmatrix}168 y^{(5)} y^{(7)} y^{(9)} - 189 y^{(5)} y^{(8)^2} - 288 y^{(7)^3} \\ +504 y^{(6)} y^{(7)} y^{(8)} - 196 y^{(6)^2} y^{(9)}\end{pmatrix}}$$

$$q_3 x_{n+1}^3 = \frac{h^3\begin{pmatrix}288 y^{(7)^2} y^{(10)} - 252 y^{(6)} y^{(8)} y^{(10)} - 720 y^{(7)} y^{(8)} y^{(9)} \\ +280 y^{(6)} y^{(9)^2} + 405 y^{(8)^3}\end{pmatrix}}{720\begin{pmatrix}168 y^{(5)} y^{(7)} y^{(9)} - 189 y^{(5)} y^{(8)^2} - 288 y^{(7)^3} \\ +504 y^{(6)} y^{(7)} y^{(8)} - 196 y^{(6)^2} y^{(9)}\end{pmatrix}}$$

Simplifying (7) by using (27) and taking $q_1 x_{n+1} = A,\ q_2 x_{n+1}^2 = B$ and $q_3 x_{n+1}^3 = C$, we obtain:

$$
\begin{aligned}
&p_0 := y_n;\\
&p_1 x_{n+1} = y_n A + h y_n^{(1)};\\
&p_2 x_{n+1}^2 = y_n B + h y_n^{(1)} A + \frac{1}{2} h^2 y_n^{(2)};\\
&p_3 x_{n+1}^3 = y_n C + h y_n^{(1)} B + \frac{1}{2} h^2 y_n^{(2)} A + \frac{1}{6} h^3 y_n^{(3)};\\
&p_4 x_{n+1}^4 = h y_n^{(1)} C + \frac{1}{2} h^2 y_n^{(2)} B + \frac{1}{6} h^3 y_n^{(3)} A + \frac{1}{24} h^4 y_n^{(4)};\\
&p_5 x_{n+1}^5 = \frac{1}{2} h^2 y_n^{(2)} C + \frac{1}{6} h^3 y_n^{(3)} B + \frac{1}{24} h^4 y_n^{(4)} A + \frac{1}{120} h^5 y_n^{(5)};\\
&p_6 x_{n+1}^6 = \frac{1}{6} h^3 y_n^{(3)} C + \frac{1}{24} h^4 y_n^{(4)} B + \frac{1}{120} h^5 y_n^{(5)} A + \frac{1}{720} h^6 y_n^{(6)};\\
&p_7 x_{n+1}^7 = \frac{1}{24} h^4 y_n^{(4)} C + \frac{1}{120} h^5 y_n^{(5)} B + \frac{1}{720} h^6 y_n^{(6)} A + \frac{1}{5040} h^7 y_n^{(7)};
\end{aligned}
\tag{28}
$$

By expanding $y_{n+1} = \dfrac{\sum_{r=0}^{7} p_r x^r}{1 + \sum_{r=1}^{3} q_r x^r}$, we get:

$$
\frac{p_7 x_{n+1}^7 + p_6 x_{n+1}^6 + p_5 x_{n+1}^5 + p_4 x_{n+1}^4 + p_3 x_{n+1}^3 + p_2 x_{n+1}^2 + p_1 x_{n+1} + p_0}{q_3 x_{n+1}^3 + q_2 x_{n+1}^2 + q_1 x_{n+1} + 1}
\tag{29}
$$

Adding up the numerator and denominator, we have:

$$
y_{n+1} = \frac{\left[\begin{array}{l} y_n(1+A+B+C) + h y^{(1)}(1+A+B+C) + \frac{1}{2} h^2 y^{(2)}(1+A+B+C) + \\ \frac{1}{6} h^3 y^{(3)}(1+A+B+C) + \frac{1}{24} h^4 y^{(4)}(1+A+B+C) \\ + \frac{1}{120} h^5 y^{(5)}(1+A+B) + \frac{1}{720} h^6 y^{(6)}(1+A) + \frac{1}{5040} h^7 y^{(7)} \end{array}\right]}{1+A+B+C}
\tag{30}
$$

III. IMPLEMENTATION OF METHODS AND RESULTS

Some selected stiff initial value problems were implemented upon by our new method for the purpose of testing its performance and suitability. The results of these initial value problems were use to compare those of other existing methods in literature.

Problem 1: $y' = -1000y + e^{-2x}, \quad y(0) = 0, \quad h = 0.001$

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

Problem 2: $y' = -8y + 8x + 1, \quad y(0) = 2, \quad h = 0.1$

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

Problem 3: $y' = -21y + e^{-x}, \quad y(0) = 0, \quad h = 0.01$

Theoretical solution: $\frac{1}{20} e^{-x} - \frac{1}{20} e^{-21x}$

Table 1: Numerical result of problem1

		Y'=-1000Y+EXP(-2X) Y(0)=0 h= 0.001					
		RIM(10)		FIRKM(5)		RADAU 11A(5)	
XN	TSOL	YN	ERROR	YN	ERROR	YN	ERROR
0.001	0.00063	0.00116	1.13E-13	0.00063	5.67E-10	0.00063	4.52E-08
0.002	0.00086	0.00093	8.33E-14	0.00086	4.17E-10	0.00086	3.32E-08
0.003	0.00095	0.00095	4.60E-14	0.00095	2.30E-10	0.00095	1.83E-08
0.004	0.00098	0.00092	2.26E-14	0.00098	1.13E-10	0.00098	9.00E-09
0.005	0.00099	0.00091	1.04E-14	0.00099	5.19E-11	0.00099	4.14E-09
0.006	0.00099	0.00089	4.58E-15	0.00099	2.29E-11	0.00099	1.83E-09
0.007	0.00099	0.00087	1.97E-15	0.00099	9.83E-12	0.00099	7.84E-10
0.008	0.00099	0.00085	8.26E-16	0.00099	4.13E-12	0.00099	3.30E-10
0.009	0.00098	0.00084	3.42E-16	0.00098	1.71E-12	0.00098	1.36E-10
0.01	0.00098	0.00082	1.40E-16	0.00098	7.00E-13	0.00098	5.58E-11

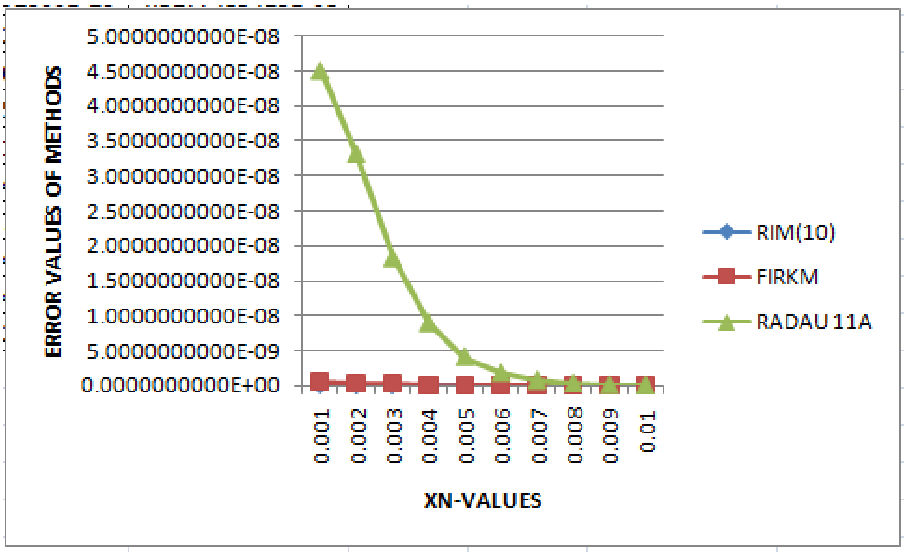

Figure 1: Error Graph of Methods (problem 1)

Table 2: Numerical result for Problem 2

		$y' = -8y + 8x + 1;\ \ y(0) = 2;\ \ h = 0.1$					
		RIM(10)		FIRKM		RADAU 11A	
XN	TSOL	YN	ERROR	YN	ERROR	YN	ERROR
0.1	0.99865793	0.99865793	2.188E-11	0.99865876	8.298E-07	0.99868731	2.938E-05
0.2	0.60379304	0.60379304	1.967E-11	0.60379378	7.457E-07	0.60381944	2.641E-05
0.3	0.48143591	0.48143591	1.326E-11	0.48143641	5.026E-07	0.48145370	1.780E-05
0.4	0.48152441	0.48152441	7.941E-12	0.48152471	3.011E-07	0.48153507	1.066E-05
0.5	0.53663128	0.53663128	4.460E-12	0.53663145	1.691E-07	0.53663727	5.989E-06
0.6	0.61645949	0.61645949	2.405E-12	0.61645959	9.119E-08	0.61646272	3.229E-06
0.7	0.70739573	0.70739573	1.261E-12	0.70739578	4.781E-08	0.70739742	1.693E-06
0.8	0.80332311	0.80332311	6.476E-13	0.80332314	2.455E-08	0.80332398	8.693E-07
0.9	0.90149317	0.90149317	3.273E-13	0.90149318	1.241E-08	0.90149361	4.394E-07
1	1.00067093	1.00067093	1.634E-13	1.00067093	6.195E-09	1.00067114	2.194E-07

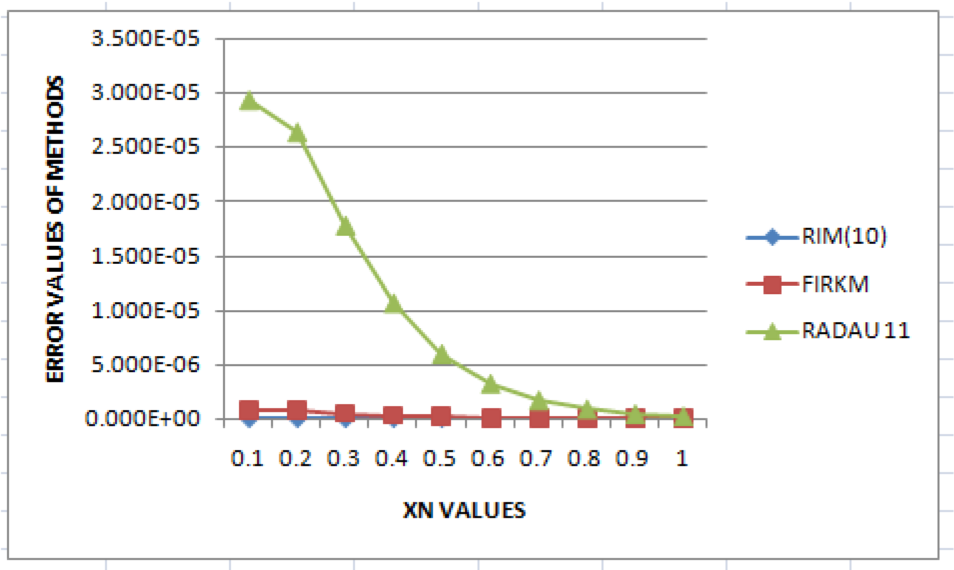

Figure 2: Error Graph of Methods (problem 2)

Table 3: Numerical result of problem 3

		Y'=-21+EXP(-X) Y(0)=0 h= 0.01					
		RIM(10)		FIRKM		RADAU 11A	
XN	TSOL	YN	ERROR	YN	ERROR	YN	ERROR
0.01	0.0090	0.0090	0.00E+00	0.0090	3.23E-11	0.00897	4.67E-10
0.02	0.0162	0.0162	6.94E-18	0.0162	5.24E-11	0.01616	7.57E-10
0.03	0.0219	0.0219	3.47E-18	0.0219	6.37E-11	0.02189	9.20E-10
0.04	0.0265	0.0265	3.47E-18	0.0265	6.89E-11	0.02646	9.94E-10
0.05	0.0301	0.0301	1.04E-17	0.0301	6.98E-11	0.03006	1.01E-09
0.06	0.0329	0.0329	6.94E-18	0.0329	6.79E-11	0.03291	9.80E-10
0.07	0.0351	0.0351	0.00E+00	0.0351	6.43E-11	0.03512	9.27E-10
0.08	0.0368	0.0368	0.00E+00	0.0368	5.96E-11	0.03684	8.58E-10
0.09	0.0381	0.0381	0.00E+00	0.0381	5.43E-11	0.03814	7.83E-10
0.1	0.0391	0.0391	6.94E-18	0.0391	4.90E-11	0.03912	7.05E-10

Figure 3: Error Graph of methods (problem 3)

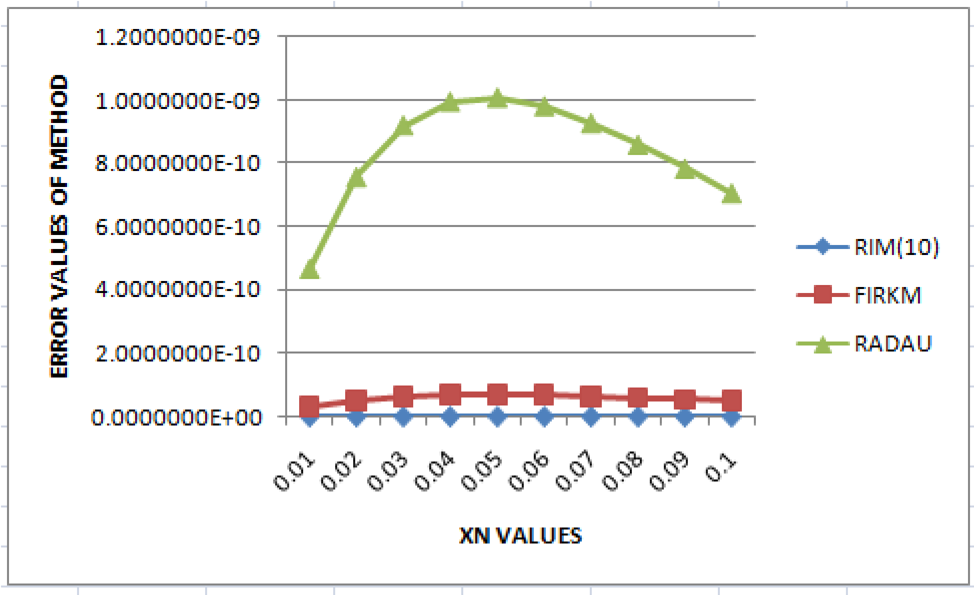

Figure 3: Error Graph of Methods (problem 3)

Note: RIM (10): Rational integrator of order 10
FIRM: Fully implicit Runge-Kutta Method of order 5
RADAU 11A: Implicit Runge-Kutta Method of order 5

IV. DISCUSSION

In deriving this method, it was acknowledged that, there are different classes of rational integrator schemes of order 10, but we consider when L > M. Then we introduced the matrix operations and the application of Crammer's rule in deriving the new rational interpolation scheme. By using MAPLE-18 software, the necessary expansions and simplifications of expressions were made with ease. A close look at the results as seen from the tables above, upon implementation on some stiff initial value problems, it was observed that the new method compared favourably well with FIRKM, RADAU II and RADAU which are in literature. In Problem 1, the results produced by these methods, in terms of the errors, were visibly low comparably. The error graphs (Figure 1-3) which give the trajectory of the errors with time, reveal that the methods performed very well in solving the problemsas their graphs are physicallyclose. However, the RADAU II method also performed equally well as the errors produced are also very low. Problems 2 and 3 which are also stiff initial value problems produced results that arefavourable. The error graphswere constructed with the help of EXCEL package.

V. CONCLUSION

The validity of the new method for the numerical solutions of stiff initial value problems have been theoretically and practically investigated and can cope very well with similar problems. In addition, the various computations displayed in the tables provided are enough proofs of the performances of the new method. Finally this article will help to reduce the rigors in the solutions of stiff initial value problems in Ordinary Differential Problems, and it is worthwhile to encourage further research-articles in similar areas of study.

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