ON THE DERIVATION OF A NEW FIFTH-ORDER IMPLICIT RUNGE-KUTTA SCHEME FOR STIFF PROBLEMS IN ORDINARY DIFFERENTIAL EQUATION

M.E. EHIEMUA¹ AND G.U. AGBEBOH

ABSTRACT. We present here, a new approach to the Radau method of solving stiff problems in Ordinary Differential Equation (ODE). This new implicit Runge-Kutta Scheme is derived for order 5, and the formular so derived was implemented, using Maple-18 package, and the results were compared with existing Radau Method. The performance of the method has improved results over those of Radau, on comparison for consistency convergence and stability.

Keywords and phrases: Radau IIA Quadrature, Taylor series, Ordinary Differential Equation and Stiff initial value problems.

2010 Mathematical Subject Classification: 65L06

1. INTRODUCTION

According to Butcher [1], initial value problems for ordinary differential equation occur very frequently in a variety of real life problems such as Control theory, Chemical engineering, Biology, Electrical and Civil engineering. Several numerical methods have been designed to solve the problems arising from the above areas of human endeavour. The ordinary differential equation:

\[ y'(x) = f(x, y(x)); (\eta) = y_0; a \leq x \leq b \]  

(1)

has often been used to profile solution, when the need arises. Such a solution given as \( y(x) \) can be a vector-valued function, going from \( \mathbb{R} \rightarrow \mathbb{R}^m \), where \( m \) is the dimension of the differential equation associated with the problem. Sometime \( y'(x) \) does not depend on \( x \), except as a parameter of \( y(x) \). In such cases (1), which is non-autonomous can be made autonomous as shown below;

\[ y'(x) = f(y(x)); (\eta) = y_0; a \leq x \leq b \]  

(2)

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Lambert [2] acknowledged that problem of this nature, consists of a first order system of Ordinary Differential Equation, together with a set of conditions which are all specified at the same initial point. The evaluation of accurate numerical methods for solving initial-value problems in terms of the rate at which the error approaches zero, when the step size $h$ approaches zero have been developed.

Butcher [3], however revealed that this characterization of accuracy is not always informative enough, because it neglects the fact that the local truncation error of any one-step or multistep method also depends on higher-order derivative of the solution. In some cases, these derivatives can be quite large in magnitude, even when the solution itself is relatively small, which requires that $h$ be made particularly small in order to achieve a reasonable accuracy. The nature of the ordinary differential equation is very important in the determination of the method of solution. For instance if the matrix is strictly lower triangular (i.e., the internal stages can be calculated without depending on the later stages), then the method is called an explicit method, if the internal stages depend not only on the previous stages but on the current stage and later stages, the method is called an implicit method.

Varah [4] acknowledged that the importance of the implicit method is seen in the fact that they can produce high orders of accuracy which are superior to those of explicit methods. This makes it more suitable for solving stiff problems. Butcher and Hojjati [5] observed that there is no agreed formal definition of what stiffness is, but stiff problem can best be recognized from the behaviour they can display when approximated by standard numerical methods. However, according to Ababneh, Ahmad and Ismail [6], stiff equations have proven to be so important to be ignored and too expensive to overpower. They are too important because they occur rather frequently in physical problems, and so expensive to overpower because of their sizes and difficulty they present to classical methods, no matter how great an improvement in computing capability becomes available.

In all computational methods, the use of a scheme for numerical solution of the initial value problem will generate errors at some stages of the computation due to the inaccuracy inherent in the formular and the arithmetic operations adopted during computer
implementation. The magnitude of the error determines the degree of accuracy and stability of the solution, thus, it is important that numerical solution approximates the exact solution and the numerical solution tends to the exact solution as the step size tends to zero as observed by Jain and Iyengar [7].

Shepley [8] iterates that if the step length used is too small, excessive computation time and round-off error results. He also observed that it is reasonable to consider the opposite case and ask whether there is any upper bound on step length. Often there is such and it is reached when the method becomes numerically unstable; i.e., the numerical solution produced, no longer corresponds quantitatively with the exact solution. According to Lambert [9], the traditional criterion for ensuring that a method is stable is called 'Absolute Stability', and this analysis is carried out by subjecting the method to a linear test equation:

$$y' = \lambda y \quad \lambda \epsilon C; \quad Re(\lambda) < 0 \quad (3)$$

Furthermore, Dekker and Verwer [10] emphasized that applying a Runge-Kutta method to Dahlquist’s test equation $y' = \lambda y$ reduces to an approximation $y_1 = R(\lambda h)y_0$. where $R(\lambda h)$ is a polynomial in the case of explicit one-step methods, and a rational function in general. However in this paper, we construct a new implicit scheme in the Radau family of order 5 that can be used to solve stiff initial value problem as will be seen in the next section.

2. DERIVATION OF METHOD

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

$$y_{n+1} - y_n = h \phi(x_n, y_n, h) \quad (4)$$

$$h \phi(x_n, y_n, h) = \sum_{r=1}^{R} b_r k_r \quad (5)$$

$$k_r = f \left( x_n + hc_r, \quad y_n + \sum_{j=1}^{R} a_{rj} k_j \right) \quad i = 1, 2, 3..R \quad (6)$$

$$c_r = \sum_{j=1}^{R} a_{rj}, \quad i = 2, 3..R \quad (7)$$

From (6), it can be seen that $k_r$ is not defined explicitly but by a set of R implicit equations. As a result, the derivation of such method is rather complicated, but can be taken care of by a procedure...
designed by Butcher. Since we are deriving a three stage method in the Radau’s family, we set \( r=3 \), and the order is \( s=(2r-1) \). For convenience, we shall be focusing on the derivatives of \( y \) alone, and the necessary Taylor series expansion is given as:

\[
\phi_T(x, y, h) = f + \frac{h}{2} \frac{f_y}{f_{yy}}(f^2 + f_{yy}) + \frac{h^3}{24}(f^3 f_{yyy} + 4f^2 f_y f_{yy} + f f_y^3)
\]

\[
+ \frac{h^4}{120}(f^4 f_{yyyy} + 7f^3 f_y f_{yyy} + 11f^2 f_y^2 f_{yy} + 4f^3 f_y^2 + f f_y^4) \tag{8}
\]

From (6), and with \( r=3 \), we obtain:

\[
k_r = (x + hc_r, y + h(ar_1 k_1 + ar_2 k_2 + ar_3 k_3)) \tag{9}
\]

Expanding (9) as a Taylor series about \( (y(x)) \), i.e., retaining all components of \( y \) derivatives only, we have:

\[
k_r = f + h((ar_1 k_1 + ar_2 k_2 + ar_3 k_3) f_y + \frac{h^2}{2} (ar_1 k_1 + ar_2 k_2 + ar_3 k_3)^2 f_{yy}
\]

\[
+ \frac{h^3}{6} (ar_1 k_1 + ar_2 k_2 + ar_3 k_3)^3 f_{yyy} + \frac{h^4}{24} (ar_1 k_1 + ar_2 k_2 + ar_3 k_3)^4 f_{yyyy} \tag{10}
\]

Now, since (9) and (10) are implicit, we cannot proceed by successive substitution as in the case of the derivation of explicit methods. In this situation, we assume, according to Butcher, that the solution for \( k_1, k_2 \) and \( k_3 \) may be expressed in the form:

\[
k_r = A_r + hB_r + h^2 C_r + h^3 D_r + h^4 E_r \tag{11}
\]

Substituting for \( k_r \) by (12) in (11), we obtain:

\[
A_r + hB_r + h^2 C_r + h^3 D_r + h^4 E_r = f + (h(ar_1(A_1 + hB_1 + h^2 C_1 + h^3 D_1)
\]

\[
+ ar_2(A_2 + hB_2 + h^2 C_2 + h^3 D_2) + ar_3(A_3 + hB_3 + h^2 C_3
\]

\[
+ h^3 D_3)) f_y + \frac{h^2}{2} ((ar_1(A_1 + hB_1 + h^2 C_1)
\]

\[
+ ar_2(A_2 + hB_2 + h^2 C_2 + ar_3(A_3 + hB_3 + h^2 C_3))^2 f_{yy}
\]

\[
+ \frac{h^3}{6} (ar_1(A_1 + hB_1) + ar_2(A_2 + hB_2) + ar_3(A_3 + hB_3))^3 f_{yyy}
\]

\[
+ \frac{h^4}{6} (ar_1 A_1 + ar_2 A_2 + ar_3 A_3)^4 f_{yyyy} \tag{12}
\]

On expanding (12) and equating power \( h \), we obtain:

\[
A_r = f
\]

\[
B_r = (A_1 ar_1 + A_2 ar_2 + A_3 ar_3) f_y
\]
Now (13) is seen to be explicit and can be solved by successive substitution. Then making use of (7), we have the following:

\[ A_r = f \]
\[ B_r = c_r f_f_y \]
\[ C_r = (c_1a_{r1} + c_2a_{r2} + c_3a_{r3})f_f_y^2 + \frac{1}{2}a_r^2f^2f_y \]
\[ D_r = ((a_{r1}(c_1a_{11} + c_2a_{12} + c_3a_{13}) + a_{r2}(c_1a_{21} + c_2a_{22} + c_3a_{23}) + a_{r3}(c_1a_{31} + c_2a_{32} + c_3a_{33}))f_f_y^3 \]
\[ + \frac{1}{2}((c_1^2a_{r1} + c_2^2a_{r2} + c_3^2a_{r3}) + 2c_r(c_1a_{r1} + c_2a_{r2} + c_3a_{r3}))f^2f_yf_y \]
\[ + \frac{1}{6}c_r^3f^3f_y \]
\[ E_r = (c_1a_{r1} + c_2a_{r2} + c_3a_{r3})(a_{r1}(c_1a_{r1} + a_{21}a_{r2} + a_{31}a_{r3})
\[ + (c_1a_{21} + c_2a_{22} + c_3a_{23})(a_{21}a_{r1} + a_{22}a_{r2} + a_{23}a_{r3})
\[ + (c_1a_{31} + c_2a_{32} + c_3a_{33})(a_{31}a_{r1} + a_{32}a_{r2} + a_{33}a_{r3}))f_y^4 \]
\[ + (a_{r1}(c_1^2a_{r1} + c_2^2a_{r2} + c_3^2a_{r3} + 2c_1(c_1a_{11} + c_2a_{12} + c_3a_{13})
\[ + a_{r2}(c_1^2a_{21} + c_2^2a_{22} + c_3^2a_{23} + 2c_2(c_1a_{21} + c_2a_{22} + c_3a_{23})
\[ + a_{r3}(c_1^2a_{31} + c_2^2a_{32} + c_3^2a_{33} + 2c_3(c_1a_{31} + c_2a_{32} + c_3a_{33}))
\[ + 2c_r(c_1a_{r1} + c_2a_{r2} + c_3a_{r3}) + 2c_r(c_1a_{r1} + c_2a_{r2} + c_3a_{r3}))f_y^2f_yf_yy^2 \]
\[ + \frac{1}{6}(c_1^3a_{r1} + c_2^3a_{r2} + c_3^3a_{r3} + 3c_r^2(c_1a_{r1} + c_2a_{r2} + c_3a_{r3}))f_yf_yf_yf_yyy \] (14)
Using (11), the expression \( \phi(x_n, y_n, h) \) defined by (5) may be written as:

\[
\phi(x_n, y_n, h) = (b_1 A_1 + b_2 A_2 + b_3 A_3) + h(b_1 B_1 + b_2 B_2 + b_3 B_3)
\]

\[
+ h^2(b_1 C_1 + b_2 C_2 + b_3 C_3) + h^3(b_1 D_1 + b_2 D_2 + b_3 D_3)
\]

\[
+ h^4(b_1 E_1 + b_2 E_2 + b_3 E_3)
\]

(15)

where the coefficients \( A_r, B_r, C_r, D_r \) and \( E_r \) for \( r=1,2,3 \) are given by (14). However, comparing (15) with the Taylor series expansion (8), we have the following equations:

\[
b_1 + b_2 + b_3 = 1
\]

\[
b_1 c_1 + b_2 c_2 + b_3 c_3 = \frac{1}{2}
\]

\[
b_1 c_1^2 + b_2 c_2^2 + b_3 c_3^2 = \frac{1}{3}
\]

\[
b_1 c_1^3 + b_2 c_2^3 + b_3 c_3^3 = \frac{1}{4}
\]

\[
b_1 c_1^4 + b_2 c_2^4 + b_3 c_3^4 = \frac{1}{5}
\]

(16)

With \( c_3 = 1 \) and using Maple-18 package to resolve (16), we obtain these values:

\[
b_1 = \left( \frac{4}{9} + \frac{\sqrt{6}}{36} \right), \quad b_2 = \left( \frac{4}{9} - \frac{\sqrt{6}}{36} \right), \quad b_3 = \frac{1}{9};
\]

\[
c_1 = \left( \frac{2}{5} + \frac{\sqrt{6}}{10} \right), \quad c_2 = \left( \frac{2}{5} - \frac{\sqrt{6}}{10} \right), \quad c_3 = 1
\]

The remaining equations with nine unknown constants were solved with the same Maple-18 package which gives the following:

\[
a_{11} = \left( \frac{3}{10} - \frac{\sqrt{6}}{60} \right), \quad a_{12} = \left( \frac{\sqrt{6}}{6} \right), \quad a_{13} = \left( \frac{1}{10} - \frac{\sqrt{6}}{20} \right)
\]

\[
a_{21} = \left( \frac{6}{125} - \frac{29\sqrt{6}}{750} \right), \quad a_{22} = \left( \frac{27}{50} - \frac{43\sqrt{6}}{300} \right), \quad a_{23} = \left( -\frac{47}{250} + \frac{41\sqrt{6}}{500} \right)
\]

\[
a_{31} = \left( \frac{33}{40} - \frac{11\sqrt{6}}{120} \right), \quad a_{32} = \left( -\frac{3}{8} + \frac{7\sqrt{6}}{24} \right), \quad a_{33} = \left( \frac{11}{20} - \frac{\sqrt{6}}{5} \right)
\]

which can be put in Butcher array as:
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\[
\begin{pmatrix}
\frac{2}{10} + \sqrt{6} & 3 - \frac{\sqrt{6}}{10} & \frac{\sqrt{6}}{6} & \frac{1}{10} - \frac{\sqrt{6}}{20} \\
\frac{2}{10} - \frac{\sqrt{6}}{10} & 6 - \frac{29\sqrt{6}}{50} & 27 - \frac{43\sqrt{6}}{300} & -\frac{47}{250} + \frac{41\sqrt{6}}{500} \\
\frac{1}{10} & 125 - \frac{75\sqrt{6}}{300} & 50 - \frac{30\sqrt{6}}{100} & 11 - \frac{\sqrt{6}}{5} \\
& 33 - \frac{11\sqrt{6}}{120} & -3 + \frac{7\sqrt{6}}{24} & \\
& & & 1
\end{pmatrix}
\]

The Radau 11A quadrature has the formula as:

\[
a_{11} = \left( \frac{11}{45} - \frac{7\sqrt{6}}{360} \right) \quad a_{12} = \left( \frac{37}{225} - \frac{169\sqrt{6}}{1800} \right) \quad a_{13} = \left( -\frac{2}{225} + \frac{\sqrt{6}}{75} \right)
\]

\[
a_{21} = \left( \frac{37}{225} + \frac{169\sqrt{6}}{1800} \right) \quad a_{22} = \left( \frac{11}{45} + \frac{7\sqrt{6}}{360} \right) \quad a_{23} = \left( -\frac{2}{225} + \frac{\sqrt{6}}{75} \right)
\]

\[
a_{31} = \left( \frac{4}{9} - \frac{\sqrt{6}}{36} \right) \quad a_{32} = \left( \frac{4}{9} + \frac{\sqrt{6}}{36} \right) \quad a_{33} = \frac{1}{9}
\]

which can also be put in Butcher array as:

\[
\begin{pmatrix}
\frac{2}{10} - \frac{\sqrt{6}}{10} & \frac{11}{45} - \frac{7\sqrt{6}}{360} & \frac{37}{225} - \frac{169\sqrt{6}}{1800} & -\frac{2}{225} + \frac{\sqrt{6}}{75} \\
\frac{2}{10} + \frac{\sqrt{6}}{10} & 37 + \frac{169\sqrt{6}}{1800} & \frac{11}{45} + \frac{7\sqrt{6}}{360} & -\frac{2}{225} - \frac{\sqrt{6}}{75} \\
\frac{1}{10} & 225 + \frac{169\sqrt{6}}{1800} & \frac{4}{9} + \frac{\sqrt{6}}{36} & \frac{4}{9} + \frac{\sqrt{6}}{36} \\
& \frac{4}{9} - \frac{\sqrt{6}}{36} & \frac{4}{9} + \frac{\sqrt{6}}{36} & \frac{4}{9}
\end{pmatrix}
\]

So the new formular becomes:

\[
y_{n+1} - y_n = h \left( \left( \frac{4}{9} + \frac{\sqrt{6}}{36} \right) k_1 + \left( \frac{4}{9} - \frac{\sqrt{6}}{36} \right) k_2 + \left( \frac{1}{9} \right) k_3 \right)
\]

3. STABILITY ANALYSIS OF METHOD

The stability of the above method, through Cramer’s rule is a rational polynomial:

\[
R(z) = \frac{\text{det}(I - zA + zeb^T)}{\text{det}(I - zA)} \quad (17)
\]

where \( b = (b_1, b_2, ... b_s) \), \( A = (a_{ij})_{i,j=1}^s \), \( e = (1, 1, 1...1) \)

Simplifying (17), and substituting the values of our new method; \((a_{ij})_{i,j=1}^s\) for \( s = 3 \), we obtain, after simplifying the resulting rational function:

\[
R(z) = 1 + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 + \frac{1}{120}z^5 \quad (18)
\]

We note at this point that the stability function of \( s \)-stage Radau method, given by \((s - 1, s)\), is the Pade approximation to the exponential function \( e^z \). Hence the stability region can also be constructed by using the rational
function given by:

\[ R(z) = \frac{P_k z}{P_m z} = \frac{\sum_{i=0}^{k} \frac{k!}{(k-1)!} \frac{(m+k-1)!z^i}{(m+k)!i!}}{\sum_{i=0}^{k} \frac{m!}{(m-1)!} \frac{(m+k-1)!(-z)^i}{(m+k)!i!}} \]  \hspace{1cm} (19)

where \( k = s - 1 \) and \( m = s \), in this case \( s = 3 \) i.e., the number of stages for the Radau’s method is 3

\[ R(z) = \left( \frac{1 + \frac{2}{5}z + \frac{1}{20}z^2}{1 - \frac{3}{5}z + \frac{3}{20}z^2 - \frac{1}{60}z^3} \right) \]  \hspace{1cm} (20)

\[ R(z) = 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 + \frac{1}{120}z^5 \]  \hspace{1cm} (21)

And with the help of MATLAB, the region of Absolute Stability (RAS) is given in figure 1. However, in figure 2, when the roots of

![Region of absolute stability for order five Runge-Kutta methods](image)

**Fig. 1.** Stability region of method.

(18) are plotted on Figure 1, we observed that the five roots of our
Fig. 2. Absolute stability of method.

method are within the region of absolute stability: The above is a clear indication that the method is Absolutely Stable.

4. IMPLEMENTATION OF METHOD

In order to ascertain the suitability of our method, the solution of some stiff initial value problems were determined by the method, in comparison with other existing Radau implicit method, of the same order.

Problem 1: \( y' = -30y; \quad y(0) = 1; \quad 0 \leq x \leq 1; \) with theoretical solution \( e^{-30x} \)

Problem 2. \( y' = -8y + 8x + 1; \quad y(0) = 2; \quad 0 \leq x \leq 1; \) with theoretical solution \( x + 2e^{-8x} \)
### TABLE 1: \( y' = -30y; y(0) = 1; 0 \leq x \leq 1 \) Agam and Yahaya (2014)

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### TABLE 2: \( y' = -8y + 8x + 1; y(0) = 2; 0 \leq x \leq 1 \) Agam and Yahaya (2014)

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</table>

### 5. ERROR ANALYSIS OF METHOD

![Fig. 3. Error analysis of Problem 1.](image-url)
DISCUSSION

In deriving the above method, we decided to assume an autonomous situation where only the derivatives of 'y' were considered. This implies that instead of having the 17 order conditions to be satisfied, it was reduced to 12 conditions, which made the derivative less costly. These 12 conditions were eventually compared with the coefficients of the expanded Taylor series for order 5, to arrive at the new method. We also observed that from Tables 1 and 2 above, the results from the new method proved to be better than that in literature. The plots 1 and 2, showing error values against the x-values for the two problems, revealed that the errors involved in Radau 11A method are higher, when compared with the new method. However, this new method is very effective in solving linear initial value problems, whether stiff or non-stiff in nature with good results that are improvement over those of Radau II. This is a clear indication that the new method is reliable, consistent and stable.

CONCLUSION

Through the approach presented in this paper, the new method can be extended to solve higher order differential equations. The method requires less work with little cost and possesses a gain in efficiency with no overlapping of results. We can also say that a stiff differential equation is numerically unstable when the step size is extremely small. Moreover, stiff differential equations are characterized as those whose exact solution has a term of the form $e^{-z}$ where 'z' is a large positive constant. From tables 1 and 2, it can be seen that the new method outperformed
over the existing implicit formulas in terms of accuracy and convergence, as evident by the decrease in error.

REFERENCES


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