A Simplified Derivation and Analysis of Fourth Order Runge Kutta Method

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ABSTRACT
The derivation of fourth order Runge-Kutta method involves tedious computation of many unknowns and the detailed step by step derivation and analysis can hardly be found in many literatures. Due to the vital role played by the method in the field of computation and applied science/engineering, we simplify and further reduce the complexity of its derivation and analysis by exploring some possibly well-known works and propose a step by step derivation of the method. We have also shown the stability region graphically

Keywords: Fourth order Runge Kutta Method, Derivation, Stability Analysis

1. INTRODUCTION
Runge-Kutta formulas are among the oldest and best understood schemes in numerical analysis. However, despite the evolution of a vast and comprehensive body of knowledge, it continues to be a source of active research [7]. Runge-Kutta methods provide a popular way to solve the initial value problem for a system of ordinary differential equations [11]:

$$y' = f(x,y),\ a \le x \le b,\ y(a) = y_0$$

with a given step length h through the interval $[a,b]$, successively producing approximations y_n to y_{n+1}. We deal exclusively with the step by step derivation and the stability analysis of the fourth order Runge-Kutta Method. For a thorough coverage of the derivation and analysis the reader is referred to [1,2,3,4,5].

The paper has the following structure: section 2 presents mathematical formulation and derivation, Section 3 presents the analysis and section 4 presents the conclusion.

2. MATHEMATICAL FORMULATION AND DERIVATION
We begin by defining the function as in [1,2,3,4,5 and 6]

$$y_{n+1} = y_n + h\phi(x,y,h)$$

Where $\phi(x,y,h) = \sum_{i=1}^{s} b_i k_i$

$$k_1 = f(x,y)$$
$$k_i = f(x + c_i h, y_n + h\sum_{j=1}^{i-1} a_{ij}k_j),\quad i = 2,3,\ldots,i-1$$
$$c_i = \sum_{j=1}^{i-1} a_{ij}$$

$$y_{n+1} = y_n + h(b_1k_1 + b_2k_2 + b_3k_3 + b_4k_4)$$
$$k_1 = f(x,y)$$
$$k_2 = f(x + c_2h, y_n + ha_{21}k_1)$$
$$k_3 = f(x + c_3h, y_n + h(a_{31}k_1 + a_{32}k_2))$$
$$k_4 = f(x + c_4h, y_n + h(a_{41}k_1 + a_{42}k_2 + a_{43}k_3))$$

The functions are expanded using a Taylor series expansion for function of two variables. To get the unknowns, we use the fourth order coefficients of order 4

$$\tau_1^{(1)} = \sum_i b_i - 1$$
$$\tau_1^{(2)} = \sum_i b_i c_i - \frac{1}{2}$$
$$\tau_1^{(3)} = \frac{1}{2}\sum_i b_i c_i^2 - \frac{1}{6}$$
$$\tau_2^{(3)} = \sum_{ij} b_i a_{ij} c_j - \frac{1}{6}$$
$$\tau_1^{(4)} = \frac{1}{6}\sum_i b_i c_i^3 - \frac{1}{24}$$
$$\tau_2^{(2)} = \sum_{ij} b_i c_i a_{ij} c_j - \frac{1}{8}$$
$$\tau_3^{(4)} = \frac{1}{2}\sum_{ij} b_i a_{ij} c_j^2 - \frac{1}{24}$$
$$\tau_4^{(4)} = \sum_{ij} b_i a_{ij} a_{jk} c_k - \frac{1}{24}$$

Setting the coefficients to zero, we have

$$b_1 + b_2 + b_3 + b_4 = 1 \tag{1}$$

$$b_2c_2 + b_3c_3 + b_4c_4 = \frac{1}{2} \qquad (2)$$

$$b_2c_2^2 b_3c_3^2 + b_4c_4^2 = \frac{1}{3} \qquad (3)$$

$$b_3c_3a_{32}c_2 + b_4c_4a_{42}c_2 + b_4c_4a_{43}c_3 = \frac{1}{8} \qquad (6)$$

$$b_3a_{32}c_2^2 + b_4a_{42}c_2^2 + b_4a_{43}c_3^2 = \frac{1}{12} \qquad (7)$$

$$b_4a_{43}a_{32}c_2 = \frac{1}{24} \qquad (8)$$

We use the simplifying assumptions by Butcher:

$$\sum_{i=1}^{s} b_i a_{ij} = b_i(1-c_j), \quad j = 2,3,4 \qquad (9)$$

Which affect the expression for $\tau_2^{(3)}, \tau_3^{(4)}$ and $\tau_4^{(4)}$. i.e.

$$\tau_2^{(3)} = \tau_1^{(2)} - 2\tau_1^{(3)}$$

$$\tau_3^{(4)} = \tau_1^{(3)} - 3\tau_1^{(4)}$$

$$\tau_4^{(4)} = \tau_1^{(2)} - 2\tau_1^{(3)} - \tau_2^{(4)}$$

Now using equation (9) for $j = 2,3 \text{ and } 4$ we have:

$$b_3a_{32} + b_4a_{42} = b_2(1-c_2) \qquad \text{(i)}$$

$$b_4a_{43} = b_3(1-c_3) \qquad \text{(ii)}$$

$0 = b_4(1-c_4)$ respectively. (iii)

Now when $j = 4$ in (iii), $c_4 = 1$ and $b_4 \neq 0$ for a four stage method.

We substitute $c_4 = 1$ in equations 2, 3 and 5 and solve for b_2, b_3 and b_4 simultaneously. Therefore equations 2, 3 and 5 becomes

$$b_2c_2 + b_3c_3 + b_4 = \frac{1}{2}$$

$$b_2c_2^2 b_3c_3^2 + b_4 = \frac{1}{3}$$

$$b_2c_2^3 + b_3c_3^3 + b_4 = \frac{1}{4}$$

Using crammer's rule, we first find the determinant of the coefficient matrix

$$b_3a_{32}c_2 + b_4a_{42}c_2 + b_4a_{43}c_3 = \frac{1}{6} \qquad (4)$$

$$b_2c_2^3 + b_3c_3^3 + b_4c_4^3 = \frac{1}{4} \qquad (5)$$

$$D = \begin{vmatrix} c_2 & c_3 & 1 \\ c_2^2 & c_3^2 & 1 \\ c_2^3 & c_3^3 & 1 \end{vmatrix} = -c_2c_3(c_2-1)(c_2-c_3)(c_3-1)$$

To solve for b_2

$$D_{b_2} = \begin{vmatrix} \frac{1}{2} & c_3 & 1 \\ \frac{1}{3} & c_3^2 & 1 \\ \frac{1}{4} & c_3^3 & 1 \end{vmatrix} = \frac{-c_3(c_3-1)(2c_3-1)}{12}$$

$$\therefore b_2 = \frac{D_{b_2}}{D} = \frac{-c_3(c_3-1)(2c_3-1)}{12} \div -c_2c_3(c_2-1)(c_2-c_3)(c_3-1) = \frac{1-2c_3}{12c_2(1-c_2)(c_3-c_2)}$$

To solve for b_3

$$D_{b_3} = \begin{vmatrix} c_2 & \frac{1}{2} & 1 \\ c_2^2 & \frac{1}{3} & 1 \\ c_2^3 & \frac{1}{4} & 1 \end{vmatrix} = \frac{c_2(c_2-1)(2c_2-1)}{12}$$

$$\therefore b_3 = \frac{D_{b_3}}{D} = \frac{c_2(c_2-1)(2c_2-1)}{12} \div -c_2c_3(c_2-1)(c_2-c_3)(c_3-1) = \frac{1-2c_2}{12c_3(c_3-c_2)(1-c_3)}$$

To solve for b_4

$$D_{b_4} = \begin{vmatrix} c_2 & c_3 & \frac{1}{2} \\ c_2^2 & c_3^2 & \frac{1}{3} \\ c_2^3 & c_3^3 & \frac{1}{4} \end{vmatrix} = \frac{-c_2c_3(c_2-c_3)(3-4c_2-4c_3+6c_2c_3)}{12}$$

$$\therefore b_4 = \frac{D_{b_4}}{D} = \frac{-c_2c_3(c_2-c_3)(3-4c_2-4c_3+6c_2c_3)}{12} \div -c_2c_3(c_2-1)(c_2-c_3)(c_3-1) = \frac{6c_2c_3-4(c_2+c_3)+3}{12(1-c_2)(1-c_3)}$$

Now to solve for a_{43} , we use equation (ii) i.e. when j=3

Hence, we have

$$\Rightarrow a_{43} = \frac{b_3(1-c_3)}{b_4} = \frac{1-2c_2}{12c_3(c_3-c_2)(1-c_3)} \times (1-c_3) \times \frac{12(1-c_2)(1-c_3)}{6c_2c_3-4(c_2+c_3)+3}$$

$$= \frac{(1-c_2)(2c_2-1)(1-c_3)}{c_3(c_2-c_3)(6c_2c_3-4(c_3+c_2))+3}$$

To solve for a_{32} and a_{42}, we use equations (i) (when j=2) and (8) i.e.

$$b_3a_{32} + b_4a_{42} = b_2(1-c_2) \qquad \text{(i)}$$

$$b_4a_{43}a_{32}c_2 = \frac{1}{24} \qquad (8)$$

$$a_{32} = \frac{1}{24c_2}\times\frac{1}{b_4}\times\frac{1}{a_{43}} = \frac{1}{24c_2}\times\frac{12(1-c_2)(1-c_3)}{6c_2c_3-4(c_3+c_2)+3}\times\frac{c_3(c_2-c_3)(6c_2c_3-4(c_3+c_2)+3)}{(1-c_2)(2c_2-1(1-c_3)}$$

$$= \frac{c_3(c_2-c_3)}{2c_2(2c_2-1)}$$

Substituting this value into (i), we have

$$a_{42} = \frac{b_2(1-c_2)-b_3a_{32}}{b_4}$$

$$= \left[\frac{1-2c_3}{12c_2(1-c_2)(c_3-c_2)}\times(1-c_2) - \frac{1-2c_2}{12c_3(1-c_3)(c_3-c_2)}\times\frac{c_3(c_2-c_3)}{2c_2(2c_2-1)}\right]\times\frac{12(1-c_2)(1-c_3)}{6c_2c_3-4(c_2+c_3)+3}$$

$$= \frac{(1-c_2)\{2(1-c_3)(1-2c_3)-(c_2-c_3)\}}{2c_2(c_2-c_3)\{6c_2c_3-4(c_2+c_3)+3)\}}$$

This solution assumes that

$$c_2 \neq 0,1, \quad c_3 \neq 0,1, \quad c_2 \neq c_3, \quad c_2 \neq \frac{1}{2}$$

We choose two free parameters $c_2 = \frac{1}{3}$ and $c_3 = \frac{2}{3}$

Substituting these values into b_4, b_3 and b_2 we have:

$$b_4 = \frac{6\left(\frac{1}{3}\right)\left(\frac{2}{3}\right)-4\left(\frac{2}{3}+\frac{1}{3}\right)+3}{12\left(1-\frac{1}{3}\right)\left(1-\frac{2}{3}\right)} = \frac{\frac{4}{3}-1}{\frac{8}{3}} = \frac{1}{8}$$

$$b_3 = \frac{1-2\left(\frac{1}{3}\right)}{12\left(\frac{2}{3}\right)\left(1-\frac{2}{3}\right)\left(\frac{2}{3}-\frac{1}{3}\right)} = \frac{\frac{1}{3}}{\frac{8}{9}} = \frac{3}{8}$$

$$b_2 = \frac{1-2\left(\frac{2}{3}\right)}{12\left(\frac{1}{3}\right)\left(1-\frac{1}{3}\right)\left(\frac{1}{3}-\frac{2}{3}\right)} = \frac{\frac{-1}{3}}{\frac{-8}{9}} = \frac{3}{8}$$

Using equation (1)

$$b_1 + b_2 + b_3 + b_4 = 1$$

$$\Rightarrow b_1 = 1 - b_2 - b_3 - b_4$$

$$= 1 - \frac{3}{8} - \frac{3}{8} - \frac{1}{8} = \frac{1}{8}$$

Also $c_2 = a_{21} = \frac{1}{3}$

Using equation (ii) (when j=3),

$$b_4a_{43} = b_3(1-c_3)$$

From equation (8) above,

$$a_{43} = \frac{b_3(1-c_3)}{b_4} = \frac{3}{8}\times\left(1-\frac{2}{3}\right)\frac{8}{1} = 1$$

Also

$$a_{42} = \frac{(1-c_2)\{2(1-c_3)(1-2c_3)-(c_2-c_3)\}}{2c_2(c_2-c_3)\{6c_2c_3-4(c_2+c_3)+3)\}}$$

$$= \frac{\left(1-\frac{1}{3}\right)\{2(1-\frac{2}{3})(1-2\times\frac{2}{3})-(\frac{1}{3}-\frac{2}{3})\}}{2\times\frac{1}{3}(\frac{1}{3}-\frac{2}{3})\{6\times\frac{1}{3}\times\frac{2}{3}-4(\frac{1}{3}+\frac{2}{3})+3)\}} = -1$$

Using equation (2) we can obtain c_4 as

$$b_4c_4 = \frac{1}{2} - b_2c_2 - b_3c_3$$

$$\Rightarrow c_4 = \frac{\frac{1}{2}-\left(\frac{3}{8}\times\frac{1}{3}\right)-\left(\frac{3}{8}\times\frac{2}{3}\right)}{\frac{1}{8}} = 1$$

Hence,

$$c_4 = a_{41} + a_{42} + a_{43}$$

$$\Rightarrow a_{41} = c_4 - a_{42} - a_{43} = 1-(-1)-1 = 1$$

Also $a_{32} = \frac{c_3(c_2-c_3)}{2c_2(2c_2-1)} = \frac{\frac{2}{3}(\frac{1}{3}-\frac{2}{3})}{2\times\frac{1}{3}(2\times\frac{1}{3}-1)} = \frac{\frac{-2}{9}}{\frac{-2}{9}} = 1$

From $c_3 = a_{31} + a_{32}$

$$\Rightarrow a_{31} = c_3 - a_{32} = \frac{2}{3} - 1 = \frac{-1}{3}$$

Finally, we know that $c_1 = a_{11} = 0$.

We have therefore determined all the unknowns in the method and the method can be written in Butcher's Tableu [3] as

0	0	0	0	0
1/3	1/3	0	0	0
2/3	-1/3	1	0	0
	1/8	3/8	3/8	1/8

Which has the form

$$y_{n+1} = y_n + \frac{h}{8}(k_1 + 3k_2 + 3k_3 + k_4)$$

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

$$k_2 = f(x_n + c_2 h, y_n + h a_{21} k_1) = f(x_n + \frac{h}{3}, y_n + \frac{h k_1}{3})$$

$$k_3 = f(x_n + c_3 h, y_n + h(a_{31}k_1 + a_{32}k_2)) = f(x_n + \frac{2}{3}h, y_n + h(-\frac{1}{3}k_1 + k_2)$$

$$k_4 = (x_n + c_4 h, y_n + h(a_{41}k_1 + a_{42}k_2 + a_{43}k_3) = f(x_n + h, y_n + h(k_1 - k_2 + k_3)$$

3. ANALYSIS OF THE METHOD

The stability polynomial is given by

$R(h) = 1 + \bar{h}b^T(I - \bar{h}A)^{-1}e$ and it is required that $R(h) < 1$ for absolute stability see [6]. Now for the Runge Kutta forth order method,

$$y_{n+1} = y_n + \frac{h}{8}(k_1 + 3k_2 + 3k_3 + k_4)$$

The Butcher's Tableu is

0	0	0	0	0
1/3	1/3	0	0	0
2/3	-1/3	1	0	0
1/8	3/8	3/8	1/8	

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & 1 & 0 & 0 \\ 1 & -1 & 1 & 0 \end{pmatrix}, \qquad I - \bar{h}A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{-\bar{h}}{3} & 1 & 0 & 0 \\ \frac{\bar{h}}{3} & -\bar{h} & 1 & 0 \\ -\bar{h} & \bar{h} & -\bar{h} & 1 \end{pmatrix},$$

$$\bar{h}b^T = \bar{h}\begin{pmatrix} \frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8} \end{pmatrix} = \begin{pmatrix} \frac{\bar{h}}{8} & \frac{3\bar{h}}{8} & \frac{3\bar{h}}{8} & \frac{\bar{h}}{8} \end{pmatrix}$$

$$\therefore \ R(\bar{h}) = 1 + \bar{h}b^T(I - \bar{h}A)^{-1}e$$

$$= 1 + \begin{pmatrix} \frac{\bar{h}}{8} & \frac{3\bar{h}}{8} & \frac{3\bar{h}}{8} & \frac{\bar{h}}{8} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{-\bar{h}}{3} & 1 & 0 & 0 \\ \frac{\bar{h}}{3} & -\bar{h} & 1 & 0 \\ -\bar{h} & \bar{h} & -\bar{h} & 1 \end{pmatrix}^{-1} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$= 1 + \begin{pmatrix} \frac{\bar{h}}{8} & \frac{3\bar{h}}{8} & \frac{3\bar{h}}{8} & \frac{\bar{h}}{8} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{\bar{h}}{3} & 1 & 0 & 0 \\ \frac{-\bar{h}}{3} + \frac{\bar{h}^2}{3} & \bar{h} & 1 & 0 \\ \bar{h} - \frac{2\bar{h}^2}{3} - \frac{\bar{h}^3}{3} & \bar{h} + \bar{h}^2 & \bar{h} & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$= 1 + \begin{pmatrix} \frac{\bar{h}}{8} + \frac{\bar{h}^2}{8} + \frac{3\bar{h}}{8}\left(\frac{-\bar{h}}{3} + \frac{\bar{h}^2}{3}\right) + \frac{\bar{h}}{8}\left(\bar{h} - \frac{2\bar{h}^2}{3} + \frac{\bar{h}^3}{3}\right) \\ \frac{3\bar{h}}{8} + \frac{3\bar{h}^2}{8} + \frac{\bar{h}}{8}\left(-\bar{h} + \bar{h}^2\right) \\ \frac{3\bar{h}}{8} + \frac{\bar{h}^2}{8} \\ \frac{\bar{h}}{8} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$= 1 + \begin{pmatrix} \frac{\bar{h}}{8} + \frac{\bar{h}^2}{8} - \frac{3\bar{h}^2}{24} + \frac{3\bar{h}^3}{24} + \frac{\bar{h}^2}{8} - \frac{2\bar{h}^3}{24} + \frac{\bar{h}^4}{24} \\ \frac{3\bar{h}}{8} + \frac{3\bar{h}^2}{8} - \frac{\bar{h}^2}{8} + \frac{\bar{h}^3}{8} \\ \frac{3\bar{h}}{8} + \frac{\bar{h}^2}{8} \\ \frac{\bar{h}}{8} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$= 1 + \frac{\bar{h}}{8} + \frac{\bar{h}^2}{8} + \frac{\bar{h}^3}{24} + \frac{\bar{h}^4}{24} + \frac{3\bar{h}}{8} + \frac{\bar{h}^2}{4} + \frac{\bar{h}^3}{8} + \frac{3\bar{h}}{8} + \frac{\bar{h}^2}{8} + \frac{\bar{h}}{8}$$

$$= 1 + \bar{h} + \frac{\bar{h}^2}{2} + \frac{\bar{h}^3}{6} + \frac{\bar{h}^4}{24}$$

For absolute stability

$$-1 < \left| 1 + \bar{h} + \frac{1}{2}\bar{h}^2 + \frac{1}{6}\bar{h}^3 + \frac{1}{24}\bar{h}^4 \right| < 1$$

Taking the RHS

$$\left| 1 + \bar{h} + \frac{1}{2}\bar{h}^2 + \frac{1}{6}\bar{h}^3 + \frac{1}{24}\bar{h}^4 \right| < 1$$

$$\bar{h} + \frac{1}{2}\bar{h}^2 + \frac{1}{6}\bar{h}^3 + \frac{1}{24}\bar{h}^4 < 0$$

Using Mathematica we get the roots as

NSolve[h+h*h/2+h*h*h/6+h*h*h*h/24==0,h]

{{h□-2.78529},{h□-0.607353-2.8719 □ },{h□-0.607353+2.8719 □ },{h□ 0.}}

We consider 3 cases as it can be found in [1]

Case 1

When λ is real and $\lambda < 0$,

The roots are -2.785 and 0

Hence the stability interval is $h \in (-2.785, 0)$.

Case 2

$$=1+\begin{pmatrix} \frac{\bar{h}}{8}+\frac{\bar{h}^2}{8}+\frac{\bar{h}^3}{24}+\frac{\bar{h}^4}{24} \\ \frac{3\bar{h}}{8}+\frac{\bar{h}^2}{4}+\frac{\bar{h}^3}{8} \\ \frac{3\bar{h}}{8}+\frac{\bar{h}^2}{8} \\ \frac{\bar{h}}{8} \end{pmatrix}\begin{pmatrix}1\\1\\1\\1\end{pmatrix}$$

When λh is pure and imaginary,

We set $\lambda = iy$ in the stability polynomial to get

$$\left|1+i(yh)-\frac{(yh)^2}{2}-i\frac{(yh)^3}{6}+\frac{(yh)^4}{24}\right|<1$$

$$\Rightarrow\left|1-\frac{(yh)^2}{2}+\frac{(yh)^4}{24}+(iyh)-i\frac{(yh)^3}{6}\right|<1$$

Let $t = yh$ and take the magnitude

$$\Rightarrow\left(1-\frac{t^2}{2}+\frac{t^4}{24}\right)^2+\left(t-\frac{t^3}{6}\right)<1$$

$$\left(1-\frac{t^2}{2}+\frac{t^4}{24}-\frac{t^2}{2}+\frac{t^4}{4}-\frac{t^6}{48}+\frac{t^4}{24}-\frac{t^6}{48}+\frac{t^8}{578}\right)+\left(t^2-\frac{t^4}{6}-\frac{t^4}{6}+\frac{t^6}{36}\right)<1$$

Simplifying, we get

$$1-\frac{t^6}{72}+\frac{t^8}{576}<1$$

$$\Rightarrow\frac{t^6}{72}+\frac{t^8}{576}<0$$

Using Mathematica to find the roots we have

```
NSolve[(-(t^6)/72)+((t^8)/576)□0,t]
{{t→-
.82843},{t→0.},{t→0.},{t→0.},{t→0.},{t→0.},{
t→0.},{t→2.82843}}
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The equation is satisfied for

$$|t|<2.82843$$

i.e. $|t|<2\sqrt{2}$

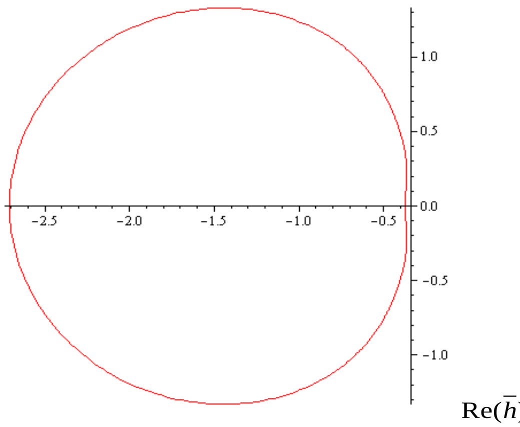
Hence the stability interval is $0<\bar{h}<2\sqrt{2}$. i.e. $\bar{h}\in(0,2\sqrt{2})$

Case 3 When λ is complex with $\mathrm{Re}(\lambda)>0$, we set $\lambda = x+iy$ in

$$\left|1+\lambda h+\frac{(\lambda h)^2}{2}+\frac{(\lambda h)^3}{6}+\frac{(\lambda h)^4}{24}\right|<1$$

and plot the boundary of the region by plotting the real and imaginary parts.

The stability region is plotted using Maple as follows



4. CONCLUSION

In this paper, we have simplified the existing derivation and analysis of the fourth order Runge-Kutta Method for easy reference to students and plot the stability region. We also reduced the complexity of the method by proposing a step by step derivation approach for better understanding to students.

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