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Implementation of a new third order weighted Runge-Kutta formula based on Centroidal Mean for solving stiff initial value problems

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Abstract

A new third order weighted Runge-Kutta formula based on Centroidal Mean(CeM) is derived and implemented. To illustrate the effectiveness of the method, a stiff problem has been chosen and compared with the classical fourth order Runge-Kutta method and the third order weighted Runge-Kutta method based on Contraharmonic Mean(CoH). The stability of the new method is analysed. The investigation undertaken in the study reveals that the third order RK method based on CeM suits very well and indicates that this method is superior compared to the other methods discussed for the stiff initial value problems.

Keywords: Runge-Kutta Method ; Centroidal Mean;Contraharmonic Mean; IVPs; Stability

INTRODUCTION

The initial value problem represented by $y' = f(x, y), y(x_0) = y_0, a \le x \le b.$ Many methods exist for the solution of IVPs in differential equations. According to Butcher (1987), it is a known fact that not all such methods have the capacity to find the solution to these IVPs. This led to the search and developed some one-step methods which can provide solution to IVPs.

Before designing our formulae, many methods were considered and motivated by the striking proposal made by Evans and Sanugi (1993), Wazwaz (1990), Ahmed and Yaacob (2005),Osama Yusuf Ababneh and Rokiah Rozita (2009) Novati (2003), Xin-Yuan Wu (1990) to study R-K method of order 3 to solve stiff problems and Wazwaz (1994), Evans and Yaccub (1996) & Murugesan et al. (2001, 2002, 2003), Sanugi and Evans (1993) & (1995), Evans and Yaccob (1995), Agbeboh, Aashikpelokhi, and Aigbedion (2007) to study R-K formulae based on variety of means. Evans and Yaakub (1996), (1998) have done the research on the weighted RK formula.

Recently, we studied about the modification of the explicit third order Runge-Kutta method using the Contrahormonic Mean (CoM) that can be used to solve Stiff Problems. In this paper, the explicit third order Runge-Kutta method based on Centroidal Mean (CeM) is introduced to solve IVPs and give a good accuracy.

A third order method for 3- stages of the (CeM) method are given in the form

$$y_{n+1} = y_n + \tfrac{h}{3}\left[\frac{k_1^{\,2} + k_1k_2 + k_2^{\,2}}{k_1 + k_2} + \frac{k_2^{\,2} + k_2k_3 + k_3^{\,2}}{k_2 + k_3}\right]$$

Where

$$k_1 = f(x_n, y_n),$$
$$k_2 = f\left(x_n + h\tfrac{2}{3}, y_n + h\tfrac{2}{3}k_1\right),$$
$$k_3 = f\left(x_n + h\tfrac{2}{3}, y_n + h\left(\tfrac{7}{9}k_1 - \tfrac{1}{9}k_2\right)\right)$$

Modified weighted Runge-Kutta Method of order three based on Centroidal Mean (MWRK3CeM)

It is possible to establish a three-stage Runge-Kutta formula based on the Centroidal Mean using the mean in the main formula which can be presented as follows:

$$y_{n+1} = y_n + h\left[\begin{array}{l} w_1\dfrac{k_1^{\,2} + k_1k_2 + k_2^{\,2}}{k_1 + k_2} \\ + w_2\dfrac{k_2^{\,2} + k_2k_3 + k_3^{\,2}}{k_2 + k_3}\end{array}\right] \quad (1)$$

where

$$k_1 = f(x_n, y_n) = f,$$
$$k_2 = f(x_n + ha_1, y_n + ha_1k_1),$$
$$k_3 = f\left(x_n + h\tfrac{2}{3}, y_n + h(a_2k_1 - a_3k_2)\right)$$

w_1 and w_2 are the weights chosen in such a way that a_1, a_2, and a_3 are parameters to be determined and $\dfrac{k_i^{\,2} + k_ik_{i+1} + k_{i+1}^{\,2}}{k_i + k_{i+1}}$ is defined as the centroidal mean. Note that for simplicity of the algebra f have been considered as a function of y only, without loss of generality. This will considerably reduce the Taylor

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Series expansions of K_i,i=1,2,3 to the following

$$k_1 = f \tag{2}$$

$$k_2 = f + ha_1 ff_y + \tfrac{1}{2} f^2 a_1^2 h^2 ff_{yy} + \tfrac{1}{6} f^3 h^3 a_1^3 f_{yyy} + \ldots \tag{3}$$

$$k_3 = f + h(a_2 + a_3) ff_y + h^2 \left(\begin{array}{l} a_1 a_3 ffy^2 + \tfrac{1}{2}(a_2 + a_3)^2 f^2 f_{yy} + \\ h^3 (\tfrac{1}{2} a_1^2 a_3 f^2 f_y f_{yy} + a_1 a_3 (a_2 + a_3) f^2 f_y f_{yy} + \\ \tfrac{1}{6}(a_2 + a_3)^3) f^3 f_{yyy} + \ldots \end{array} \right) \tag{4}$$

Traditionally, the equations (2) to (4) would be substituted to obtain an expression of y_{n+1} in terms of the function together with the parameter a_i,i=1,2,3 and its derivatives. Since the algebra involved is the division of two series,

$$\frac{k_i^2 + k_i k_{i+1} + k_{i+1}^2}{k_i + k_{i+1}}, \text{ i=1(1)3} \tag{5}$$

Here direct substitution cannot be done. These problems are alleviated by multiplying the terms across with the common denominator $(k_1+k_2)(k_2+k_3)$ and can be written as

$$y_{n+1} = y_n + \tfrac{Upper}{Lower} \tag{6}$$

with

$$Upper = 2h(w_1(k_1^2 + k_1 k_2 + k_2^2)(k_2 + k_3) + w_2(k_2^2 + k_2 k_3 + k_3^2)(k_1 + k_2))$$

And

$$Lower = 3(k_1 + k_2)(k_2 + k_3)$$

Taylor Series expansion of y (x_{n+1}) may be written as

$$Taylor = y_n + hf + \tfrac{1}{2} h^2 ff_y + \tfrac{1}{6} h^3 (ff_y^2 + f^2 f_{yy}) + \tfrac{1}{24} h^4 (f^3 f_{yyy} + 4 f^2 f_y f_{yy} + ff_y^2) + \ldots \tag{7}$$

Since the error of the method can be measured using the expression

$$Error = y(x_{n+1}) - y_{n+1}$$

We get,

$$Error = Taylor - \tfrac{Upper}{Lower}$$

We could rewrite the above as,

$$ErrorXLower = TaylorXLower - Upper \tag{8}$$

Comparing the coefficients of the same terms in (8) upto the term h^3, we get the following equations of conditions:

$$hf^3 : 12 w_1 + 12 w_2 - 12 = 0 \tag{9}$$

$$h^2 f^3 f_y : 18 a_1 w_1 + 18 a_1 w_2 + 6 a_2 w_1 + 12 a_2 w_2 + 6 a_3 w_1 + 12 a_3 w_2 - 12 a_1 - 6 a_2 - 6 a_3 - 6 = 0 \tag{10}$$

$$h^3 f^3 f_y^2 : 10 a_1^2 w_1 + 10 a_1^2 w_2 + 6 a_1 a_2 w_1 + 12 a_1 a_3 w_1 + 4 a_2^2 w2 + 4 a_3^2 w_2 + 10 a_1 a_2 w_2 + 22 a_1 a_3 w_1 + 8 a_2 a_3 w_2 - 3 a_1^2 - 3 a_1 a_2 - 9 a_1 a_3 - 6 a_1 - 3 a_2 - 3 a_3 = 0 \tag{11}$$

$$h^3 f^4 f_{yy} : 9 a_1^2 w_1 + 3 a_2^2 w_1 + 3 a_3^2 w_1 + 6 a_2 a_3 w_1 + 9 a_1^2 w_2 + 6 a_2^2 w_2 + a_3^2 w_2 + 12 a_2 a_3 w_2 - 6 a_1^2 - 3 a_2^2 - 3 a_3^2 - 6 a_2 a_3 - 2 = 0 \tag{12}$$

Solving the equations (9)-(12) using MATLAB we obtained a set of parameters and weights shown below

$$w_1 = \tfrac{1}{2}, w_2 = \tfrac{1}{2}, a_1 = \tfrac{2}{3}, a_2 = \tfrac{7}{9}, a_3 = -\tfrac{1}{9}$$

The third order centroidal mean RK formula MWRK3CeM can be represented by,

$$\begin{aligned} k_1 &= f(x_n, y_n), \\ k_2 &= f\left(x_n + h\tfrac{2}{3}, y_n + h\tfrac{2}{3} k_1\right), \\ k_3 &= f\left(x_n + h\tfrac{2}{3}, y_n + h\left(\tfrac{7}{9} k_1 - \tfrac{1}{9} k_2\right)\right) \end{aligned} \tag{13}$$

$$y_{n+1} = y_n + \tfrac{h}{3}\left[\frac{k_1^2 + k_1 k_2 + k_2^2}{k_1 + k_2} + \frac{k_2^2 + k_2 k_3 + k_3^2}{k_2 + k_3}\right] \tag{14}$$

When

$$w_1 = \tfrac{1}{4}, w_2 = \tfrac{3}{4}, a_1 = \tfrac{4+\sqrt{2}}{7}, a_2 = \tfrac{128-38\sqrt{2}}{189},$$

$$a_3 = \tfrac{-20+2\sqrt{2}}{189}$$

$$\begin{aligned} k_1 &= f(x_n, y_n), \\ k_2 &= f\left(x_n + h\tfrac{4+\sqrt{2}}{7}, y_n + h\tfrac{4+\sqrt{2}}{7} k_1\right), \\ k_3 &= f\left(x_n + h\tfrac{108-36\sqrt{2}}{189}, y_n + h\left(\tfrac{128-38\sqrt{2}}{189} k_1 + \tfrac{-20+2\sqrt{2}}{189} k_2\right)\right) \end{aligned} \tag{15}$$

$$y_{n+1} = y_n + \tfrac{2h}{3}\left[\tfrac{1}{4}\frac{k_1^2 + k_1 k_2 + k_2^2}{k_1 + k_2} + \tfrac{3}{4}\frac{k_2^2 + k_2 k_3 + k_3^2}{k_2 + k_3}\right] \tag{16}$$

Stability Analysis

To check on the stability when the weights $w_1 = \tfrac{1}{2}, w_2 = \tfrac{1}{2}$, the equations in (13) & (14) are substituted into the simple test equation $y' = \lambda y$ and it yields,

$$k_1 = f(x_n, y_n) = \lambda y_n \tag{17}$$

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$$k_2 = f\left(x_n + h\tfrac{2}{3}, y_n + h\tfrac{2}{3}\lambda y_n\right)$$

$$= \lambda y_n (1 + \tfrac{2}{3} h\lambda) \quad (18)$$

$$k_3 = f\left(x_n + h\tfrac{2}{3}, y_n + h\left(\tfrac{7}{9}k_1 - \tfrac{1}{9}k_2\right)\right)$$

$$= \lambda y_n (1 + \tfrac{16}{27} h\lambda)$$

(19)

Substituting (17), (18), & (19)in (14),and letting $z = h\lambda$, We obtain the simplified equation

$$y_{n+1} = y_n + \frac{h}{3}\left[\frac{\lambda^2 {y_n}^2 + \lambda^2 {y_n}^2 (1+\frac{2}{3}z) + \lambda^2 {y_n}^2 (1+\frac{2}{3}z)^2}{\lambda y_n (1+(1+\frac{2}{3}z))}\right] + \frac{\lambda^2 {y_n}^2 (\frac{1}{9}(9+4z^2+12z) + \frac{1}{81}(32z^2+102z+81) + \frac{1}{729}(256z^2+864z+70))}{\frac{\lambda y_n}{81}(102z+162)}$$

$$y_{n+1} = y_n + zy_n\left[\left[\frac{4z^2+18z+27}{18z+54}\right] + \left[\frac{868z^2+2754z+2187}{2754z+4374}\right]\right]$$

which yield the stability polynomial

$$y_{n+1} = y_n\left[1 + z\left[\left[\frac{4z^2+18z+27}{18z+54}\right] + \left[\frac{868z^2+2754z+2187}{2754z+4374}\right]\right]\right]$$

or in more simplified form,

$$y_{n+1} = y_n\left[R(z)\right]$$

where

$$R(z) = 1 + z\left[\left[\frac{4z^2+18z+27}{18z+54}\right] + \left[\frac{868z^2+2754z+2187}{2754z+4374}\right]\right]$$

$$R(z) = 1 + z + 0.4815\, z^2 + 0.0187\, z^3 - 0.0063\, z^4 + 0.0021z^5 + 0.0508z^6 + 0.0321z^7$$

To check on the stability when the weights $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}$, the equations in (15) & (16) are substituted into the simple test equation $y' = \lambda y$ and it yields,

$$k_1 = f(x_n, y_n) = \lambda y_n \quad (20)$$

$$k_2 = f\left(x_n + h\tfrac{4+\sqrt{2}}{7}, y_n + h\tfrac{4+\sqrt{2}}{7}k_1\right),$$

$$= \lambda y_n (1 + \tfrac{4+\sqrt{2}}{7} h\lambda) \quad (21)$$

$$k_3 = f\left(\begin{array}{l} x_n + h(\frac{128-38\sqrt{2}}{189} + \frac{-20+2\sqrt{2}}{189}), \\ y_n + h\left(\frac{128-38\sqrt{2}}{189}\lambda y_n + \frac{-20+2\sqrt{2}}{189}\lambda y_n (1 + \frac{4+\sqrt{2}}{7}h\lambda)\right)\end{array}\right)$$

$$= \lambda y_n (1 + \tfrac{680-264\sqrt{2}}{1323} h\lambda) \quad (22)$$

Substituting (20), (21), & (22) in (16),and letting $z = h\lambda$ we obtain the simplified equation

$$y_{n+1} = y_n + \frac{h}{3}\left[\frac{\lambda^2 {y_n}^2 + \lambda^2 {y_n}^2 (1+\frac{4+\sqrt{2}}{7}z) + \lambda^2 {y_n}^2 (1+\frac{4+\sqrt{2}}{7}z)^2}{\lambda y_n (1+(1+\frac{4+\sqrt{2}}{7}z))}\right] + \left[\frac{\lambda^2 {y_n}^2 (1+\frac{4+\sqrt{2}}{7}z)^2 + \lambda^2 {y_n}^2 (1+\frac{4+\sqrt{2}}{7}z)(1+(\frac{680-264\sqrt{2}}{1323})z) + (1+(\frac{680-264\sqrt{2}}{1323})z)^2}{\lambda y_n ((1+\frac{4+\sqrt{2}}{7}z) + 1 + (\frac{680-264\sqrt{2}}{1323})z)}\right]$$

$$y_{n+1} = y_n + zy_n\left[\left[\frac{(18+8\sqrt{2})z^2 + (84+21\sqrt{2})z + 147}{42(14+(4+\sqrt{2})z)}\right] + \left[\frac{1+\frac{z^2}{49}(18+8\sqrt{2}) + \frac{z}{7}(18+8\sqrt{2}) + (1+\frac{4+\sqrt{2}}{7}z)(1+(\frac{680-264\sqrt{2}}{1323})z) + (1+(\frac{680-264\sqrt{2}}{1323})z)^2}{(4+2z(\frac{4+\sqrt{2}}{7}+(\frac{680-264\sqrt{2}}{1323}))}\right]\right]$$

which yield the stability polynomial

$$y_{n+1} = y_n\left[1 + z\left[\left[\frac{(18+8\sqrt{2})z^2 + (84+21\sqrt{2})z + 147}{42(14+(4+\sqrt{2})z)}\right] + \left[\frac{1+\frac{z^2}{49}(18+8\sqrt{2}) + \frac{z}{7}(18+8\sqrt{2}) + (1+\frac{4+\sqrt{2}}{7}z)(1+(\frac{680-264\sqrt{2}}{1323})z) + (1+(\frac{680-264\sqrt{2}}{1323})z)^2}{(4+2z(\frac{4+\sqrt{2}}{7}+(\frac{680-264\sqrt{2}}{1323}))}\right]\right]\right]$$

or in more simplified form,

$$y_{n+1} = y_n\left[R(z)\right]$$

where

$$R(z) = \left[1 + z\left[\frac{(18+8\sqrt{2})z^2 + (84+21\sqrt{2})z + 147}{42(14+(4+\sqrt{2})z)}\right] + z\left[\frac{1+\frac{z^2}{49}(18+8\sqrt{2}) + \frac{z}{7}(18+8\sqrt{2}) + (1+\frac{4+\sqrt{2}}{7}z)(1+(\frac{680-264\sqrt{2}}{1323})z) + (1+(\frac{680-264\sqrt{2}}{1323})z)^2}{(4+2z(\frac{4+\sqrt{2}}{7}+\frac{680-264\sqrt{2}}{1323}))}\right]\right]$$

$$= 1 + z + 0.4736z^2 + 0.0308z^3 - 0.01403z^4$$
$$+ 0.0065z^5 + 0.0231z^6 + 0.0145z^7$$

Given R, we can determine its stability region by noting ,by the maximum modulus principal, that it is the region enclosed by the set of points for which IR(z)I=1. For a particular point z on the boundary of the stability region there must exists an angle θ for which $R(z) = \exp(i\theta)$ and we can trace out this boundary by solving this polynomial equation for values of θ in (0,2π)

Various points on the boundary are located by taking θ in steps of $\frac{2\pi}{n}$ from 0 to 2π and then invoking a procedure point which is supposed to print a point x+iy on this boundary.

The method used to solve for Z=x+iy by the Newton – Raphson method, taking the value at the previous angle as the initial approximation and taking zero as the initial approximation for θ=0. The algorithm is designed so that it will deal with a polynomial

$R(z) = a[0] + a[1]z + a[2]z^2 + ... + a[s]z^s$. The variable eps is the required accuracy.

Numerical Experiments

The MWRK3CeM methods for two different weights are tested on the example of system of stiff differential equation to check on the accuracy of this method. We will comparing the new method by the existing classical fourth order Runge-Kutta method and the new third order weighted Runge- kutta method based on Contraharmanic Mean with the step size h=0.01.Where the fourth order classical Runge-Kutta method uses the formula

$$k_1 = hf(t_n, x_n, y_n),$$
$$k_2 = hf\left(t_n + \tfrac{h}{2}, x_n + \tfrac{k_1}{2}, y_n + \tfrac{m_1}{2}\right),$$
$$k_3 = hf\left(t_n + \tfrac{h}{2}, x_n + \tfrac{k_2}{2}, y_n + \tfrac{m_2}{2}\right),$$
$$k_4 = hf(t_n + h, x_n + k_3, y_n + m_3)$$

Where

$$y_{n+1} = y_n + \tfrac{(k_1 + 2(k_2 + k_3) + k_4)}{6}$$

And the new third order weighted Runge- Kutta method based on Contraharmanic Mean for the weights $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}$ uses the formula

$$k_1 = f(t_n, x_n, y_n),$$
$$k_2 = f\left(t_n + h\tfrac{4-\sqrt{2}}{7}, x_n + h\tfrac{4-\sqrt{2}}{7}k_1, y_n + h\tfrac{4-\sqrt{2}}{7}m_1\right),$$
$$k_3 = f\left(t_n + h\tfrac{12+4\sqrt{2}}{21}, x_n + h\tfrac{12+4\sqrt{2}}{21}k_2, y_n + h\tfrac{12+4\sqrt{2}}{21}k_2\right),$$

where

$$y_{n+1} = y_n + \tfrac{h}{4}\left[\tfrac{1}{4}\frac{k_1^{\,2} + k_2^{\,2}}{k_1 + k_2} + \tfrac{3}{4}\frac{k_2^{\,2} + k_3^{\,2}}{k_2 + k_3}\right]$$

Example: Consider the System of Stiff Differential Equation

$$y'(t) = y(t)$$
$$y'(t) = -100y(t) - 0.9999x(t), y(1) = -1$$

With the exact solution

$$x(t) = (\tfrac{9999}{9998})\exp(-0.01)t - (\tfrac{1}{9998})\exp(-99.99)t$$
$$y(t) = (-\tfrac{99.99}{9998})\exp(-0.01)t + (\tfrac{99.99}{9998})\exp(-99.99)t$$

The absolute error of the explicit MWRK3CeM method, h=0.01 on an example compared to MCHW-RK3 method when the weights $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}$ and the Classical RK4.

Table: 1

SYSTEM OF STIFF DIFFERENTIAL EQUATIONS						
	MCeMW-RK3		MCHW-RK3		RK4	
T	X	Y	X	Y	X	Y
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.0000e+000	9.851825e-003	9.851825e-005	2.5053e-003	2.5019e-005	9.902479e-003	9.902479e-005
2.0000e+000	9.753797e-003	9.753797e-005	4.8809e-003	4.8809e-005	9.803948e-003	9.803948e-005
3.0000e+000	9.656745e-003	9.656745e-005	1.2175e-002	1.2175e-004	9.706397e-003	9.706397e-005
4.0000e+000	9.560659e-003	9.560659e-005	1.9379e-002	1.9379e-004	9.609816e-003	9.609816e-005
5.0000e+000	9.465529e-003	9.465529e-005	2.6492e-002	2.6492e-004	9.514197e-003	9.514197e-005

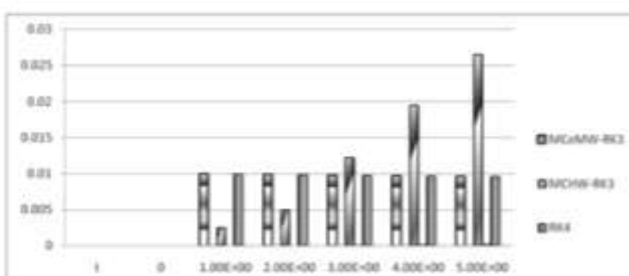
The absolute error of the explicit MWRK3CeM method, h=0.01 on an example compared to MCHW-RK3 method when the weights $w_1 = \frac{1}{2}, w_2 = \frac{1}{2}$ .and the classical RK4

Table: 2

SYSTEM OF STIFF DIFFERENTIAL EQUATIONS						
	MCeMW-RK3		MCHW-RK3		RK4	
T	X	y	X	Y	x	Y
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
1.0000e+000	9.874997e-003	9.874997e-005	2.4177e-003	2.4172e-005	9.902479e-003	9.902479e-005
2.0000e+000	9.776739e-003	9.776739e-005	4.9683e-003	4.9683e-005	9.803948e-003	9.803948e-005
3.0000e+000	9.679459e-003	9.679459e-005	1.2262e-002	1.2262e-004	9.706397e-003	9.706397e-005
4.0000e+000	9.583147e-003	9.583147e-005	1.9466e-002	1.9466e-004	9.609816e-003	9.609816e-005
5.0000e+000	9.487793e-003	9.487793e-005	2.6579e-002	2.6579e-004	9.514197e-003	9.514197e-005

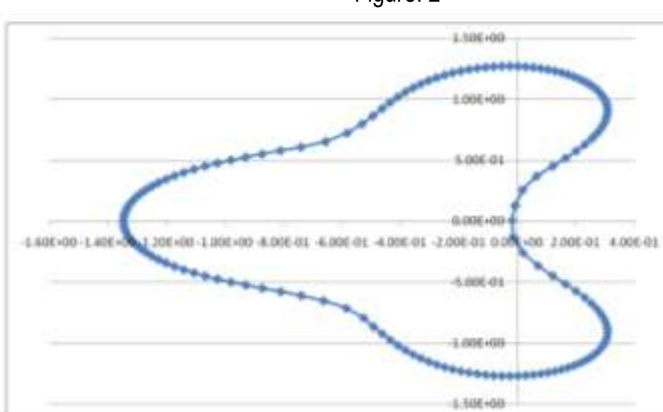
Error graph of the stiff problem to MWRK3CeM, MCHW-RK3 methods when the weights $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}$ and the classical RK4 taking h = 0.01

Figure: 1



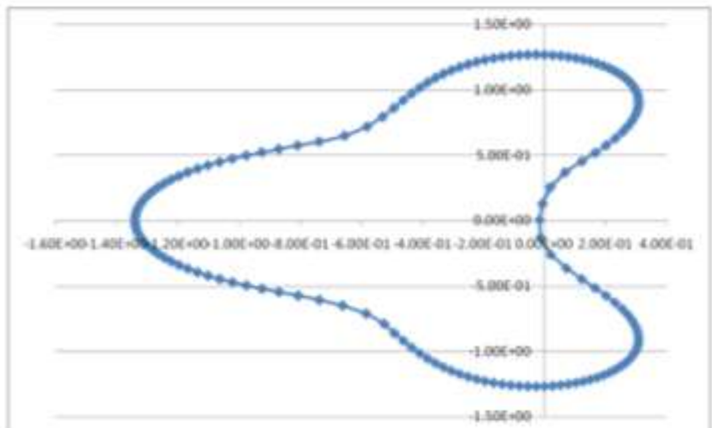
The stability region of the MWRK3CeM $\left(\frac{1}{2}, \frac{1}{2}\right)$

Figure: 2



The stability region of the MWRK3CeM $\left(\frac{1}{4}, \frac{3}{4}\right)$

Figure: 3



DISCUSSION AND CONCLUSION:

The research done in this paper shows the possibility of constructing an explicit three-stage third order Centroidal mean Runge-Kutta formula to solve initial value problems . With the purpose of verifying the accuracy of the above said method an example of the stiff differential equation is taken and compared with the existing Classical RK4 and MCHW-RK3 methods. Table 1 and table 2 shows the absolute error of an example for the methods when

h = 0.01 when the weights are taken as $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}$ and $w_1 = \frac{1}{2}, w_2 = \frac{1}{2}$ respectively. Figure 1 represents the error graph of the stiff problem to MWRK3CeM, MCHW-RK3 , RK4 methods taking h=0.01 when the weights $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}$. Figures 2, 3 show the stability of the new MWRK3CeM method for different weights. The results show that there is an excellent accuracy of MWRK3CeM method using the step size h=0.01 for the system of stiff differential equations when compared to both MCHW-RK3 and RK4. For the system of stiff differential equations MWRK3CeM method gives more accuracy when the weights are taken as $w_1 = \frac{1}{4}, w_2 = \frac{3}{4}$ than the weights are taken as $w_1 = \frac{1}{2}, w_2 = \frac{1}{2}$. But both the methods are equally good.

From this discussion it is clearly confirmed that the new proposed MWRK3CeM method is appropriate for the system of stiff differential equation.

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