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Weighted Block Runge-Kutta Method for Solving Stiff Ordinary Differential Equations

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ABSTRACT

In this paper, weighted block Runge-Kutta (WBRK) method is derived for solving stiff ordinary differential equations (ODEs). Implementation of weights on the method and its stability region are shown. Numerical results of the WBRK method are presented and compared with the existing methods to prove the ability of the proposed method to solve stiff ODEs. The results show that the WBRK method has better accuracy than the comparing methods.

Keywords: Runge-Kutta method, weights, block method, stiff ODEs, Centroidal mean.

1. Introduction

A differential equation (DE) is an equation that involves one or more derivatives of some unknown functions. Many problems in engineering, physical and social sciences are reduce to quantifiable form through the process of mathematical modelling which involved DEs. An example of modelling a real world problem using DE is in population change which is affected by births, death, immigration, and emigration. In most applicable situations, the exact solution of the DEs that model the problem is too complicated to be solved analytically. Hence, it is convenient to make approximations of the solution by numerical methods.

There are two main approaches for numerical techniques, namely, linear multistep method (LMM), and the one-step method. Adams method is widely known for the LMM users, while RK method has been used extensively in a one-step algorithm. The interest of using the one-step method, specifically RK method, over LMM is due to the advantage of RK method which requires no additional starting values and ability to readily change the steplength during computation. We use the explicit RK method which exhibits smaller computational cost than the implicit one which obtained through Taylor series as shown in Lambert (1973). Previously, it is known that implicit RK is more suitable to solve stiff problems however, Wu (1998) developed a sixth order A-stable explicit one-step method to show that an explicit method is efficient to solve stiff problems too.

A weighted fifth-order RK formulas for second-order differential equations proposed by Evans and Yaakub (1998) is an extension from Evans and Yaakub (1996) who introduced a new fifth order five stage Arithmetic Mean (AM) weighted RK (WRK) method. The implementation of weights on the method improves the efficiency of the method to solve problem of DEs. RK formula based on variety of means for solving the system of initial value problems (IVPs) as suggested by Murugesan et al. (2001) is then extended by Pushpam and Dhayabaran (2011) to solve stiff non-linear system. Ababneh and Rozita (2009) derived a weighted third order RK method based on Contraharmonic Mean (WRK3CoM) that is suitable to solve stiff problem. Sharmila and Amirtharaj (2011) used a modified weighted RK method based on Centroidal Mean (MWRK3CeM) for solving stiff IVPs, and shows that it is more effective than WRKCoM.

Many researchers especially mathematicians have extended the existing method or developed a new method to solve the problem efficiently by reducing the computational cost and obtained smaller error. The method that is capable to evaluate functions in block of several of steps at once instead of one step at a time is a block method. Milne (1953) introduced a block method for numerical solutions of the first and higher order ODEs to be used as a starting value for a predictor-corrector algorithm. A block diagonally implicit RK (BDIRK) method by Cash (1983) is used to solve stiff and non-stiff problems of IVPs in ODEs. Then, Cash (1985) extended the method to form a block embedded explicit RK method which has the characteristics of standard explicit RK formula except for the function evaluation that is done in several steps at once. The derivation of BDIRK is also available in Rahim (2004). Majid and Suleiman (2007) developed a four-point fully implicit block method fo solving first order ODEs by using variable stepsize. A block backward differentiation formula (BBDF) of variable step for solving stiff ODEs proposed by Ibrahim et al. (2007) have better accuracy with reduction of total steps and lesser computational time when compared with classical BDF by Suleiman (1979). The BBDF method is then improved in terms of its accuracy by several researchers, such as Yatim et al. (2011), Zawawi et al. (2012) and Ismail et al. (2014). Technique of partitioning introduced by Othman et al. (2007) which is based on BBDF proposed by Ibrahim et al. (2007) is proved to reduce the cost of the iteration scheme.

In this paper, we consider the following first order ODE of the form

$$\mathbf{y'} = A\mathbf{y} + \phi(x) \tag{1}$$

where $\mathbf{y}^T = (y_1, y_2, ..., y_m)$ and A is an $m \times m$ matrix with eigenvalues λ_t, $t = 1, 2, .., m$. According to Lambert (1993),

Definition 1: The system of first order ODE as shown in 1 is said to be stiff if
1) $Re(\lambda_t) < 0, t = 1, 2, ..., m$.
2) $max_t|Re(\lambda_t)| >> min_t|Re(\lambda_t)|$ where λ_t are the eigenvalues of A.

As shown in Lambert (1973), stiffness is dependent only on the large ratio of the magnitudes of the negative real parts of the largest eigenvalue to that of the smallest one. Stiffnes ratio is defined as $S = \frac{max_t|Re(\lambda_t)|}{min_t|Re(\lambda_t)|}$, hence stiff problem has $S >> 1$.

Derivation of the WBRK method is shown in Section 2. The stability of WBRK is provided in Section 3. Section 4 presents the numerical results of the proposed method when tested with problems of stiff ODEs. Finally, we conclude findings of this research in Section 5.

2. Derivation of WBRK

Murugesan et al. (2001) extended the RK method based on variety of means which include AM, Geometric Mean (GM), Harmonic Mean (HaM), Heronian Mean (HeM), Root Mean Square (RMS), CeM, and CoM for solving system of IVPs. As shown in the paper, general form of CeM in terms of AM and GM used to derive the WBRK method is presented as follows.

$$\frac{4(AM)^2-(GM)^2}{3(AM)}$$

or in general form of

$$\frac{2}{3}\Big(\frac{x_1^2+x_1x_2+x_2^2}{x_1+x_2}\Big) \tag{2}$$

Since WBRK method is based on third order RK, we will use the MWRK3CeM method by Sharmila and Amirtharaj (2011) as a foundation of our proposed method. Standard form of MWRK3CeM with implementation of weights is shown as follows

$$y_{n+1}=y_n+\frac{2}{3}h\Big(w_1\frac{k_1^2+k_1k_2+k_2^2}{k_1+k_2}+w_2\frac{k_2^2+k_2k_3+k_3^2}{k_2+k_3}\Big) \tag{3}$$

where

$$\begin{aligned}
k_1 &= f(x_n,y_n),\\
k_2 &= f(x_n+a_1h, y_n+ha_1k_1),\\
k_3 &= f(x_n+(a_2+a_3)h, y_n+h(a_2k_1+a_3k_2)).
\end{aligned}$$

Equation (3) can be transformed into a block method by integrates forward over a step $2h$ on the Taylor series expansion of k_i with $i=1,2,3$ which yields

$$\begin{aligned}
k_1 =&f,\\
k_2 =&f+2ha_1ff_y+2h^2f^2a_1^2f_{yy}+\frac{4}{3}h^3f^3a_1^3f_{yyy},\\
k_3 =&f+2h(a_2+a_3)ff_{yy}+4h^2\Big(a_1a_3ff_y^2+\frac{1}{2}(a_2+a_3)^2f^2f_{yy}\Big)+\\
&8h^2\Big(\frac{1}{2}a_1^2a_3f^2f_yf_{yy}+a_1a_3(a_2+a_3)f^2f_yf_{yy}+\frac{1}{6}(a_2+a_3)^3f^3f_{yyy}\Big)
\end{aligned} \tag{4}$$

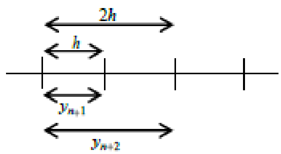

Figure 1: Block explicit RK method of constant stepsize

Figure 1 shows the computation works of WBRK method.

By substituting Equation (4) into Equation (3), we obtain an expression y_{n+2} in terms of the function with parameter a_i for $i = 1, 2, 3$, and its derivatives. The formula obtained involves a division of two series as follows

$$\sum_{i=1}^{2} \frac{k_i^2 + k_i k_{i+1} + k_{i+1}}{k_i + k_{i+1}} \tag{5}$$

These problems can be solved by cross multiplying the series with the common denominator $(k_1 + k_2)(k_2 + k_3)$. Hence, it can be written as

$$y_{n+1} = y_n + \frac{U}{L} \tag{6}$$

with

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

and

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

The Taylor series expansion of $y(x_{n+2})$, T, can be written as such

$$T = y_n + (2h)f + \tfrac{1}{2}(2h^2 f f_y + \tfrac{1}{6}(2h)^3(f f_y^2 + f^2 f_{yy})$$

The error of the method, E, is measured by the following expression

$$E = y(x_{n+2}) - y_{n+1}.$$

This yields

$$E = T - \frac{U}{L}. \tag{7}$$

Then, by comparing the coefficients of like terms for Equation (7) up to term h^3 yields the following

$$hf^3 : 24w_1 + 24w_2 - 24 = 0 \tag{8}$$

$$\begin{aligned} h^2f^3f_y :& 72w_1a_1 + 24w_1a_2 + 24w_1a_3 + 72w_2a_1 + 48w_2a_2 + 48w_2a_3 \\ & - 48a_1 - 24a_2 - 24a_3 - 24 = 0 \end{aligned} \tag{9}$$

$$\begin{aligned} h^3f^3f_y^2 :& 80w_1a_1^2 + 80w_2a_1^2 + 32w_2a_2^2 + 32w_2a_3^2 + 48w_1a_1a_2 + \\ & 96w_1a_1a_3 + 80w_2a_1a_2 + 176w_2a_1a_3 + 64w_2a_2a_3 - 24a_1^2 - \\ & 24a_1a_2 - 72a_1a_3 - 48a_1 - 24a_2 - 24a_3 - 16 = 0 \end{aligned} \tag{10}$$

$$\begin{aligned} h^3f^4f_{yy} :& 72w_1a_1^2 + 24w_1a_2^2 + 24w_1a_3^2 + 72w_2a_1^2 + 48w_2a_2^2 + 48w_2a_3^2 + \\ & 48w_1a_2a_3 + 96w_2a_2a_3 - 48a_1^2 - 24a_2^2 - 24a_3^2 - 48a_2a_3 - 16 \\ & = 0 \end{aligned} \tag{11}$$

Equations (8), (9), (10) and (11) are solved for the chosen weights to obtain a set of parameters. Following Evans and Yaakub (1998), the set of weights chosen must satisfy $\sum_{i=1}^{2} = 1$. Hence, we randomly choose weights, $w_1 = w_2 = \frac{1}{2}$. On that account, we obtain the following set of parameters

$$a_1 = \tfrac{2}{3}, a_2 = -\tfrac{2}{9}, a_3 = \tfrac{8}{9}.$$

By substituting the weights and the set of parameters into Equation (3) results the following equation

$$\begin{aligned} y_{n+1} &= y_n + \frac{1}{3}h\Big(w_1\frac{k_1^2 + k_1k_2 + k_2^2}{k_1 + k_2} + w_2\frac{k_2^2 + k_2k_3 + k_3^2}{k_2 + k_3}\Big), \\ y_{n+2} &= y_n + \frac{2}{3}h\Big(w_1\frac{k_1^2 + k_1k_2 + k_2^2}{k_1 + k_2} + w_2\frac{k_2^2 + k_2k_3 + k_3^2}{k_2 + k_3}\Big), \end{aligned} \tag{12}$$

where

$$\begin{aligned} k_1 &= f(x_n, y_n), \\ k_2 &= f\Big(x_n + \frac{2}{3}h, y_n + \frac{2}{3}hk_1\Big), \\ k_3 &= f\Big(x_n + \frac{2}{3}h, y_n + h(-\frac{2}{9}k_1 + \frac{8}{9}k_2)\Big). \end{aligned} \tag{13}$$

This completes the derivation.

3. Stability of WBRK

In this section, we analyze the stability of WBRK method. As referred in Rahim (2004), absolute stability can be defined as follows.

Definition 2: By letting $z = h\lambda$, then $R(z)$ is known as the stability function of the method. Hence $y_n \to 0$ as $n \to 0$ if and only if

$$|R(z)| < 1 \tag{14}$$

and the method is absolutely stable for those value of z for which Equation (14) holds. The region R_A of the complex $z-$plane which the equation holds is the region of absolute stability.

In order to construct the stability region of the method, we have to find the stability polynomial. By considering the following test equation,

$$\begin{aligned} y' =& f(x, y) \\ =& \lambda y \end{aligned} \tag{15}$$

We substitute Equation (15) into Equation (13) which gives us the following

$$\begin{aligned} k_1 &= f(x_n, y_n) = \lambda y_n, \\ k_2 &= f\Big(x_n + \frac{2}{3}h, y_n + \frac{2}{3}hk_1\Big) = \lambda y_n\Big(1 + \frac{2}{3}h\lambda\Big), \\ k_3 &= f\Big(x_n + \frac{2}{3}h, y_n + h(-\frac{2}{9}k_1 + \frac{8}{9}k_2)\Big) = \lambda y_n\Big(1 + \frac{2}{3}h\lambda + \frac{16}{27}h^2\lambda^2\Big). \end{aligned} \tag{16}$$

By substituting Equation (16) into Equation (12), and letting $\frac{y_{n+1}}{y_n} = R(h\lambda)$, we obtain the following

$$\begin{aligned} R(h\lambda) =& (13122 + 26244h\lambda + 26487h^2\lambda^2 + 16848h^3\lambda^3 + 6804h^4\lambda^4 + \\ & 1920h^5\lambda^5 + 256h^6\lambda^6)\frac{1}{162(3 + h\lambda)(27 + 18h\lambda + 8h^2\lambda^2)} \end{aligned} \tag{17}$$

Then, we let $z = h\lambda$ into Equation (17) to obtain

$$\begin{aligned} R(z) =& (13122 + 26244z + 26487z^2 + 16848z^3 + 6804z^4 + \\ & 1920z^5 + 256z^6)\frac{1}{162(3 + z)(27 + 18z + 8z^2)} \end{aligned} \tag{18}$$

Equation (18) is known as stability function or stability polynomial of the method. Clearly, $y_n \to 0$ as $n \to 0$ if and only if when $|R(z)| < 1$ which satisfies the condition mentioned in **Definition 2**. Hence, the WBRK method is absolute stable. By using MAPLE, the stability regions of the method are presented as follows.

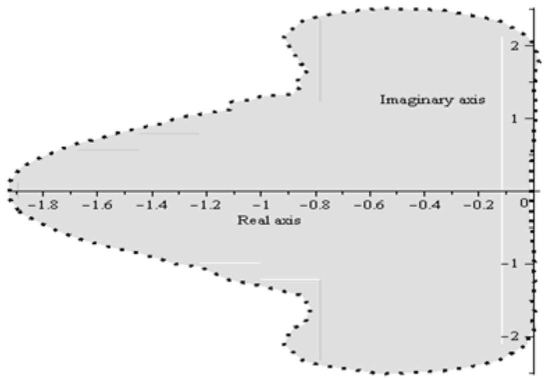

Figure 2: Stability region of WBRK method

Figure 2 shows that the stability regions of the method lies inside the closed region. We find the interval of absolute stability of the method by using MAPLE which is approximately [-1.94,0]. According to Burden et al. (2015), a method can be applied effectively to a stiff equation only if $h\lambda$ is in the region of absolute stablity of the method.

4. Numerical Results

In this section, we present the numerical results of WBRK method to check on the accuracy of the method. The method is tested with three ODEs of stiff type and we compare the maximum error (MAXE) and computational time (TIME) of the method with MWRK3CeM as shown in Sharmila and Amirtharaj (2011) and the third order RK method in Lambert (1973).

Table 1-3 tabulate the results while Figure 3-8 illustrate the graphical form between the Log(MAXE) versus Log(h) and Log(TIME).

The methods are tested with stepsize, h=0.01, 0.0001, and 0.000001. λ shows the eigenvalue(s) of the following test problems.

Problem 1:
$y' = -15y, \qquad y(0) = 1, \qquad 0 \leq x \leq 1$
with exact solution
$y = e^{-15x}, \qquad \lambda = -15$
Source: Berland (2007).

Problem 2:
$y' = -20(y - x) + 1, \qquad y(0) = 1, \qquad 0 \leq x \leq 10$
with exact solution
$y = e^{-20x} + x, \qquad \lambda = -20$
Source: Gear (1971).

Problem 3:
$x' = 42y - 43x, \qquad x(0) = 8, \qquad 0 \leq x \leq 1$
$y' = -8y + 7x, \qquad y(0) = 1,$
with exact solution
$x = 2e^{-t} + 6e^{-50t}, \qquad \lambda = -1$
$y = 2e^{-t} - e^{-50t}, \qquad \lambda = -50$
Source: Huang (2005).

Table 1: Comparison of WBRK of weights, $w_1 = w_2 = \frac{1}{2}$ with MWRK3CeM and RK3 for solving Problem 1

Stepsize, h	Method	MAXE(y_{n+1})
	WBRK	7.111898824E-05
10^{-2}	MWRK3CeM	1.536057468E-03
	RK3	2.184967940E-02
	WBRK	5.949740700E-11
10^{-4}	MWRK3CeM	1.381024156E-07
	RK3	1.842618470E-04
	WBRK	7.438494265E-15
10^{-6}	MWRK3CeM	1.380451309E-11
	RK3	1.839429394E-06

Table 2: Comparison of WBRK of weights, $w_1 = w_2 = \frac{1}{2}$ with MWRK3CeM and RK3 for solving Problem 2

Stepsize, h	Method	MAXE(y_{n+1})
10^{-2}	WBRK	2.271357959E-04
	MWRK3CeM	2.803610572E-03
	RK3	2.840716293E-02
10^{-4}	WBRK	2.966545146E-08
	MWRK3CeM	2.430198235E-07
	RK3	2.250360654E-04
10^{-6}	WBRK	7.684324288E-10
	MWRK3CeM	7.684324288E-10
	RK3	2.244994309E-06

Table 3: Comparison of WBRK of weights, $w_1 = w_2 = \frac{1}{2}$ with MWRK3CeM and RK3 for solving Problem 3

Stepsize, h	Method	MAXE(y_{n+1})
10^{-2}	WBRK	2.467754126E-02
	MWRK3CeM	1.331770888E-01
	RK3	2.966907540E-01
10^{-4}	WBRK	6.934759966E-08
	MWRK3CeM	9.247600947E-06
	RK3	1.859830420E-03
10^{-6}	WBRK	1.375306535E-10
	MWRK3CeM	9.214335961E-10
	RK3	1.849920277E-05

From Table 1-3, we can observed that the WBRK method obtained smaller MAXE when compared with the MWRK3CeM method and RK3 method. In comparison of the stepsize used, it shows that stepsize, h=0.000001 obtained smaller MAXE.

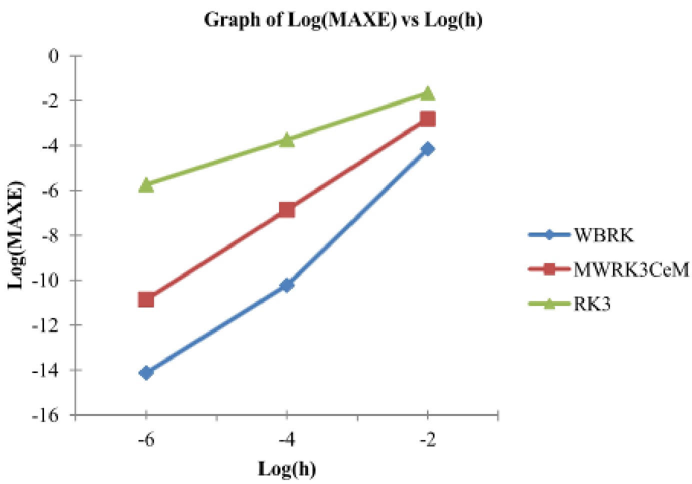

Figure 3: Graph of Log(MAXE) vs Log(h) of WBRK method is compared with MWRK3CeM and RK3 for solving Problem 1

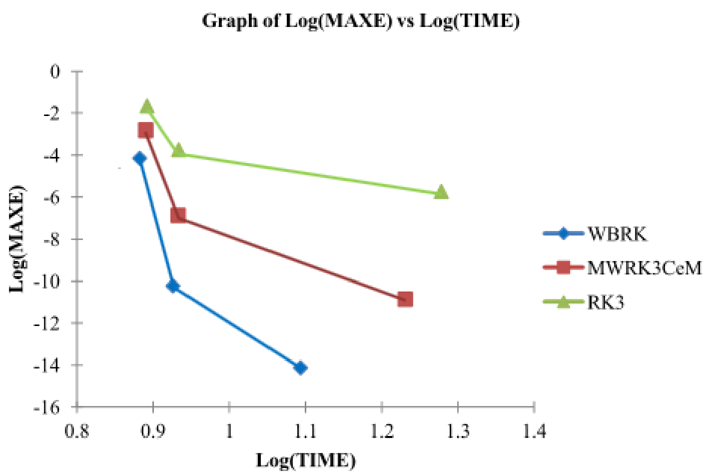

Figure 4: Graph of Log(MAXE) vs Log(TIME) of WBRK method is compared with MWRK3CeM and RK3 for solving Problem 1

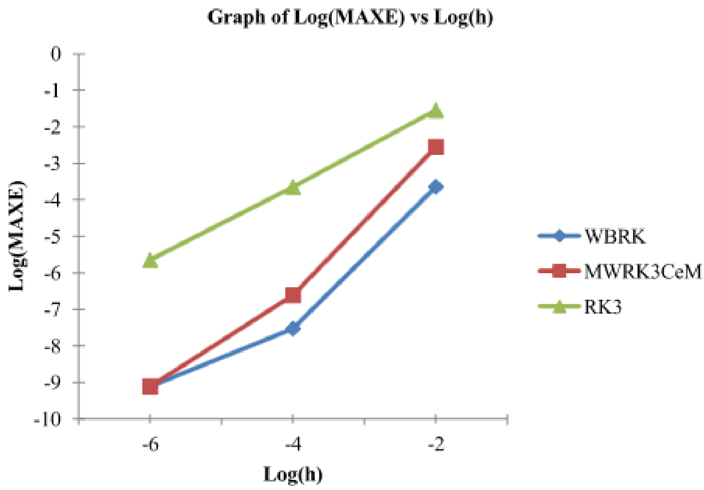

Figure 5: Graph of Log(MAXE) vs Log(h) of WBRK method is compared with MWRK3CeM and RK3 for solving Problem 2

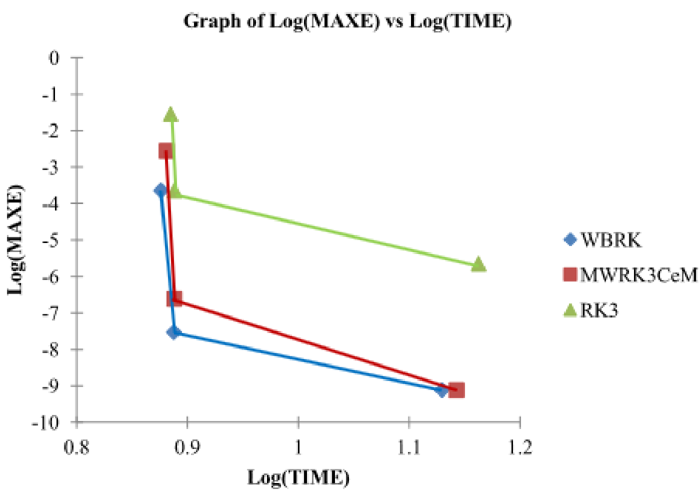

Figure 6: Graph of Log(MAXE) vs Log(TIME) of WBRK method is compared with MWRK3CeM and RK3 for solving Problem 2

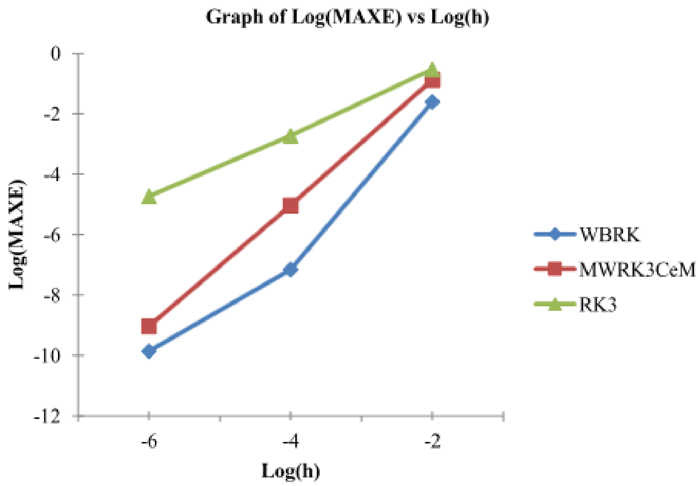

Figure 7: Graph of Log(MAXE) vs Log(h) of WBRK method is compared with MWRK3CeM and RK3 for solving Problem 3

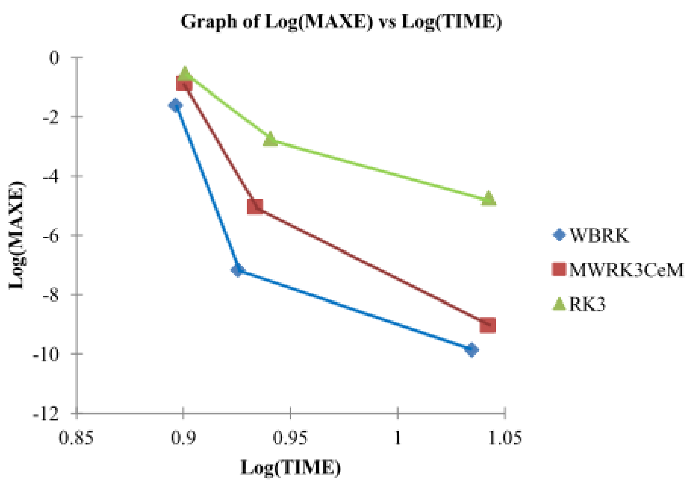

Figure 8: Graph of Log(MAXE) vs Log(TIME) of WBRK method is compared with MWRK3CeM and RK3 for solving Problem 3

Figure 3-8 illustrate the efficiency of WBRK method based on its execution time and stepsize used when compared with the MWRK3CeM and the RK3 method.

5. Conclusion

The derivation of WBRK based on CeM for solving stiff ODEs is shown in this paper. From the stability regions of the WBRK method, we can conclude that the method is absolute stable. The numerical results prove that WBRK method has better accuracy than the comparing methods. The results also show better accuracy when smaller stepsize is used. From the efficiency graph shown in Figure 3-8, we can observe that WBRK method performs better in terms of its execution time when compared with the MWRKCeM and the RK3 method. Hence, we can conclude that WBRK method can serve as an alternative solver for solving stiff ODEs problems.

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