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A New Class of Rational Multistep Methods for Solving Initial Value Problem

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ABSTRACT

There exists initial value problem whose solution possesses singularity. Studies show that conventional numerical method such as multistep method fail woefully near the singular point when solving problem whose solution possesses singularity. This is because a multistep method is based on the local representation of polynomial of the theoretical solution of an initial value problem. Therefore, a natural step would appear to be the replacement of the polynomial function for a multistep method, by a rational function due to its smooth behaviour in the neighbourhood of singularity. In this paper, we have developed a new class of two-step numerical methods that are based on rational functions in solving general initial value problem and problem whose solution possesses singularity. These new methods are called rational multistep methods. The developments of these rational multistep methods, as well as the local truncation error and stability analysis for each rational multistep method are presented. We have found out that only the second order, third order and fourth order rational multistep methods are *A*-stable. Numerical experiments have showed that all newly developed rational multistep methods presented in this paper are suitable to solve general initial value problem, stiff problem and problem whose solution possesses singularity.

Keywords: rational function, rational multistep method, initial value problem, stiff problem, problem whose solution possesses singularity.

1. INTRODUCTION

Conventional numerical methods for solving general initial value problems of the form

$$y'(x)=f\left(x,y(x)\right),\ y(a)=\eta;\ y(x),f\left(x,y(x)\right)\in \mathrm{R},\ x\in[a,b]\subset \mathrm{R},\qquad (1)$$

that have been widely used nowadays are those from the class of linear multistep methods and the class of Runge-Kutta methods. Besides methods from these two classes, there are other options such as the predictor-corrector methods and hybrid methods. If the initial value problem whose solution possesses singularity, then numerical integration formulae that are based on rational functions will be much more effective. According to Lambert (1973), Van Niekerk (1988) and Ikhile (2001), conventional multistep methods that are based on the local representation of a polynomial of the theoretical solution to (1), will fail woefully near the singular points when solving problem whose solution possesses singularity. Therefore, a natural step would appear to be the replacement of the polynomial function for a multistep method, by a rational function due to its smooth behaviour in the neighbourhood of singularity (Ikhile (2001)).

The literature reviews on numerical methods that are based on rational functions, or better known as rational methods, are very fruitful but many of them focus on the developments of single-step rational methods, see the works by Lambert and Shaw (1965), Lambert (1974), Wambecq (1976), Van Niekerk (1987), Van Niekerk (1988), Ikhile (2001), Ikhile (2002), Ikhile (2004), and Ramos (2007). On the other hand, there are only a few works that focus on the developments of multistep methods that are based on rational functions, see the works by Luke *et al.* (1975), Fatunla (1982), Fatunla (1986), Okosun and Ademiluyi (2007a), Okosun and Ademiluyi (2007b), and recently, Teh *et al.* (2011). Teh *et al.* (2011) had developed a class of 2-step p-th order rational methods which based on the rational function mentioned in Van Niekerk (1988). Teh *et al.* (2011) had named these 2-step p-th order methods as RMM2(2,p) with $p = 2,3,\ldots$.

Motivated by the successful developments of RMM2(2,p), we wish to develop another new class of multistep methods which give better numerical accuracy especially in solving problem whose solution possesses singularity. Hence, the objective of this study is to develop some explicit 2-step rational methods from the rational function mentioned in Ikhile (2001). The developments of these new multistep methods have contributed to the body of knowledge as we suggest some alternatives that are more accurate compared to other existing rational methods in the previous studies.

In Section 2, we have presented some theoretical frameworks which backup the developments of some 2-step rational methods discussed in Section 3 – Section 6. Numerical experiments and comparisons are carried out in Section 7. In Section 8, we have showed the generalization of the newly developed 2-step rational methods to r-step rational methods based on the rational function mentioned in Ikhile (2001). Lastly, a conclusion is given in Section 9. Throughout this paper, we have addressed multistep methods that are based on rational functions as rational multistep methods, or in brief as RMMs.

2. THEORETICAL FRAMEWORKS OF THE NEW RATIONAL MULTISTEP METHODS

Suppose that we have solved (1) numerically up to a point x_n and have obtained a value y_n as an approximation of $y(x_n)$, which is the theoretical solution of (1). From Lambert (1973) and Lambert (1991), by the localizing assumption that no previous truncation errors have been made i.e. $y_n = y(x_n)$, we are interested in obtaining y_{n+2} as the approximation of $y(x_{n+2})$. For that purpose, we suggest an approximation to the theoretical solution $y(x_{n+2})$ of (1) given by

$$y_{n+2} = B + \frac{Ah}{1+\sum_{j=1}^{K} b_j h^j}, \quad 1+\sum_{j=1}^{K} b_j h^j \neq 0, \tag{2}$$

where B, A and b_j , $j = 1,\ldots,K$ are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$.

RMM in (2) is defined as 2-step p-th order RMM3 or in brief as RMM3(2,p) with $p = 2,3,\ldots$. With the RMM3 in (2), we associate the difference operator L defined by

$$L\left[y(x);h\right]_{\text{RMM3}} = \left(y(x+2h)-B\right)\times\left(1+\sum_{j=1}^{K} b_j h^j\right) - Ah, \tag{3}$$

where $y(x)$ is an arbitrary function, continuously differentiable on $x \in [a,b] \subset \mathrm{R}$. Expanding $y(x+2h)$ as Taylor series and collecting terms in (3) give the following general expression:

$$L\left[y(x);h\right]_{\text{RMM3}} = C_0 h^0 + C_1 h^1 + \cdots + C_K h^K + C_{K+1} h^{K+1} + \cdots. \tag{4}$$

We note that C_i , $i = 0,1,\ldots,K,K+1$ in (4) contain corresponding parameters which need to be determined in the derivation processes. Therefore, the order and local truncation errors of RMM3 based on (2) are defined as follows.

Definition 1. The difference operator (3) and the associated rational multistep method (2) are said to be of order $p = K+1$ if, in (4), $C_0 = C_1 = \cdots = C_{K+1} = 0$, $C_{K+2} \neq 0$.

Definition 2. The local truncation error at x_{n+2} of (2) is defined to be the expression $L\left[y(x_n);h\right]_{\text{RMM3}}$ given by (3), when $y(x_n)$ is the theoretical solution of the initial value problem (1) at a point x_n. The local truncation error of (2) is then

$$L\left[y(x_n);h\right]_{\text{RMM3}} = C_{K+2}h^{K+2} + O\left(h^{K+3}\right). \tag{5}$$

3. 2-STEP SECOND ORDER RMM3

In order to derive a second order RMM3, we have to take $K = 1$ in (3), expand $y(x+2h)$ into series to obtain the following expression:

$$\begin{aligned} L\left[y(x);h\right]_{\text{RMM3}} &= -B + y(x) + h\left(-A - Bb_1 + b_1 y(x) + 2y'(x)\right) \\ &\quad + h^2\left(2b_1 y'(x) + 2y''(x)\right) + h^3\left(2b_1 y''(x) + \frac{4}{3}y'''(x)\right) \\ &\quad + O\left(h^4\right). \end{aligned} \tag{6}$$

Following Definition 1 and (4), it is readily deduced that:

$$\left\{C_0 = -B + y(x), C_1 = -A - Bb_1 + b_1 y(x) + 2y'(x), C_2 = 2b_1 y'(x) + 2y''(x),\right.$$
$$\left. C_3 = 2b_1 y''(x) + \frac{4}{3}y'''(x)\right\}.$$

With $C_0 = C_1 = C_2 = 0$, we obtain a system of three simultaneous equations which has the following solutions

$$\left\{B = y(x), A = 2y'(x), b_1 = -\frac{y''(x)}{y'(x)}\right\}. \tag{7}$$

Substituting the parameters in (7) into C_3, we obtain

$$C_3 = -\frac{2y''(x)^2}{y'(x)} + \frac{4}{3}y'''(x). \tag{8}$$

When $y(x)$ is now taken as the theoretical solution of the initial value problem (1) at a point x_n i.e. $y(x) = y(x_n)$, (7) can be written as

$$\left\{B = y_n, A = 2y'_n, b_1 = -\frac{y''_n}{y'_n}\right\}, \tag{9}$$

where $y_n = y(x_n)$ and $y_n^{(m)} = y^{(m)}(x_n)$, $m = 1,2$ by the localizing assumption. By taking $K = 1$, (2) becomes

$$y_{n+2} = B + \frac{Ah}{1 + b_1 h},\ 1 + b_1 h \neq 0. \tag{10}$$

We indicate (10) based on (9) as RMM3(2,2), expressed in the form of

$$y_{n+2} = y_n + \frac{2h(y'_n)^2}{y'_n - hy''_n}. \tag{11}$$

We note that RMM3(2,2) which presented in (11), is identical to RMM2(2,2) of Teh *et al.* (2011). From Definition 2 and (8), the local truncation error (in brief as LTE) of RMM3(2,2) is given by

$$\text{LTE}_{\text{RMM3(2,2)}} = h^3\left(-\frac{2(y''_n)^2}{y'_n} + \frac{4}{3}y'''_n\right) + O(h^4), \tag{12}$$

where $y_n^{(m)} = y^{(m)}(x_n)$, $m = 1,2,3$ by the localizing assumption.

If we apply RMM3(2,2) to the Dahlquist's test equation $y' = \lambda y$, $\mathrm{Re}(\lambda) < 0$, we obtain the following difference equation

$$y_{n+2} = \frac{1+h\lambda}{1-h\lambda} y_n . \tag{13}$$

Setting $z = h\lambda$, $y_{n+2} = \xi^2$ and $y_n = \xi^0 = 1$ in (13), we obtain the following characteristic equation

$$\xi^2 - \frac{1+z}{1-z} = 0 . \tag{14}$$

The roots of (14) are

$$\xi_{(14,1)} = -\frac{\sqrt{1+z}}{\sqrt{1-z}} \text{ and } \xi_{(14,2)} = \frac{\sqrt{1+z}}{\sqrt{1-z}} .$$

By taking $z = x + \mathrm{i}y$ in the roots of (14), we have plotted the region of absolute stability of RMM3(2,2) in Figure 1.

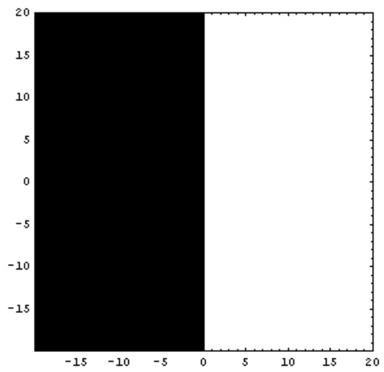

Figure 1: Stability region of RMM3(2,2).

The shaded region in Figure 1 is the region of absolute stability of RMM3(2,2), where the conditions: $\left|\xi_{(14,1)}\right| \le 1$ and $\left|\xi_{(14,2)}\right| \le 1$ are satisfied. From Figure 1, we can see that the region of absolute stability of RMM3(2,2) contains the whole left-hand half plane, which show that RMM3(2,2) is A-stable.

4. 2-STEP THIRD ORDER RMM3

In order to derive a third order RMM3, we have to take $K = 2$ in (3), expand $y(x+2h)$ into series to obtain the following expression:

$$\begin{aligned}
&L\left[y(x);h\right]_{\text{RMM3}} \\
&= -B + y(x) + h\left(-A - Bb_1 + b_1 y(x) + 2y'(x)\right) \\
&\quad + h^2\left(-Bb_2 + b_2 y(x) + 2b_1 y'(x) + 2y''(x)\right) \\
&\quad + h^3\left(2b_2 y'(x) + 2b_1 y''(x) + \frac{4}{3}y'''(x)\right) + h^4\left(2b_2 y''(x) + \frac{4}{3}b_1 y'''(x) + \frac{2}{3}y^{(4)}(x)\right) \\
&\quad + O\left(h^5\right).
\end{aligned} \tag{15}$$

Following Definition 1 and (4), it is readily deduced that:

$$\begin{aligned}
&\Big\{C_0 = -B + y(x), C_1 = -A - Bb_1 + b_1 y(x) + 2y'(x), \\
&\quad C_2 = -Bb_2 + b_2 y(x) + 2b_1 y'(x) + 2y''(x), C_3 = 2b_2 y'(x) + 2b_1 y''(x) + \frac{4}{3}y'''(x), \\
&\quad C_4 = 2b_2 y''(x) + \frac{4}{3}b_1 y'''(x) + \frac{2}{3}y^{(4)}(x)\Big\}.
\end{aligned}$$

With $C_0 = C_1 = C_2 = C_3 = 0$, we obtain a system of four simultaneous equations which has the following solutions:

$$\left\{B = y(x), A = 2y'(x), b_1 = -\frac{y''(x)}{y'(x)}, b_2 = \frac{3y''(x)^2 - 2y'(x)y'''(x)}{3y'(x)^2}\right\}. \tag{16}$$

Substituting the parameters in (16) into C_4, we obtain

$$C_4 = \frac{2y''(x)^3}{y'(x)^2} - \frac{8y''(x)\,y'''(x)}{3y'(x)} + \frac{2}{3}y^{(4)}(x). \tag{17}$$

When $y(x)$ is now taken as the theoretical solution of the initial value problem (1) at a point x_n i.e. $y(x) = y(x_n)$, (16) can be written as

$$\left\{ B = y_n, A = 2y'_n, b_1 = -\frac{y''_n}{y'_n}, b_2 = \frac{3(y''_n)^2 - 2y'_n y'''_n}{3(y'_n)^2} \right\}, \tag{18}$$

where $y_n = y(x_n)$ and $y_n^{(m)} = y^{(m)}(x_n)$, $m = 1,2,3$ by the localizing assumption. By taking $K = 2$, (2) becomes

$$y_{n+2} = B + \frac{Ah}{1 + b_1 h + b_2 h^2}, \; 1 + b_1 h + b_2 h^2 \neq 0. \tag{19}$$

We indicate (19) based on (18) as RMM3(2,3), expressed in the form of

$$y_{n+2} = y_n + \frac{6h(y'_n)^3}{3(y'_n)^2 - 3hy'_n y''_n + 3h^2(y''_n)^2 - 2h^2 y'_n y'''_n}. \tag{20}$$

From Definition 2 and (17), LTE of RMM3(2,3) is given by

$$\text{LTE}_{\text{RMM3(2,3)}} = h^4 \left(\frac{2(y''_n)^3}{(y'_n)^2} - \frac{8y''_n y'''_n}{3y'_n} + \frac{2}{3}y_n^{(4)} \right) + O(h^5), \tag{21}$$

where $y_n^{(m)} = y^{(m)}(x_n)$, $m = 1,2,3,4$ by the localizing assumption.

If we apply RMM3(2,3) to the Dahlquist's test equation $y' = \lambda y$, $\text{Re}(\lambda) < 0$, we obtain the following difference equation:

$$y_{n+2} = \frac{3 + 3h\lambda + h^2\lambda^2}{3 - 3h\lambda + h^2\lambda^2} y_n. \tag{22}$$

Setting $z = h\lambda$, $y_{n+2} = \xi^2$ and $y_n = \xi^0 = 1$ in (22), we obtain the following characteristic equation

$$\xi^2 - \frac{3+3z+z^2}{3-3z+z^2} = 0. \tag{23}$$

The roots of (23) are

$$\xi_{(23,1)} = -\frac{\sqrt{3+3z+z^2}}{\sqrt{3-3z+z^2}} \text{ and } \xi_{(23,2)} = \frac{\sqrt{3+3z+z^2}}{\sqrt{3-3z+z^2}}.$$

By taking $z = x + \mathrm{i}y$ in the roots of (23), the region of absolute stability of RMM3(2,3) is exactly the one shown in Figure 1. The shaded region in Figure 1 becomes the region of absolute stability of RMM3(2,3), where the conditions: $\left|\xi_{(23,1)}\right| \le 1$ and $\left|\xi_{(23,2)}\right| \le 1$ are satisfied. We can see that the region of absolute stability of RMM3(2,3) contains the whole left-hand half plane, which show that RMM3(2,3) is also *A*-stable.

5. 2-STEP FOURTH ORDER RMM3

In order to derive a fourth order RMM3, we have to take $K = 3$ in (3), expand $y(x+2h)$ into series to obtain the following expression

$$\begin{aligned} L\left[y(x);h\right]_{\text{RMM3}} = & -B + y(x) + h\left(-A - Bb_1 + b_1 y(x) + 2y'(x)\right) \\ & + h^2\left(-Bb_2 + b_2 y(x) + 2b_1 y'(x) + 2y''(x)\right) \\ & + h^3\left(-Bb_3 + b_3 y(x) + 2b_2 y'(x) + 2b_1 y''(x) + \frac{4}{3} y'''(x)\right) \\ & + h^4\left(2b_3 y'(x) + 2b_2 y''(x) + \frac{4}{3} b_1 y'''(x) + \frac{2}{3} y^{(4)}(x)\right) \\ & + h^5\left(2b_3 y''(x) + \frac{4}{3} b_2 y'''(x) + \frac{2}{3} b_1 y^{(4)}(x) + \frac{4}{15} y^{(5)}(x)\right) \\ & + O\left(h^6\right). \end{aligned} \tag{24}$$

Following Definition 1 and (4), it is readily deduced that

$$\begin{aligned}\{C_0 &= -B + y(x), C_1 = -A - Bb_1 + b_1 y(x) + 2y'(x),\\ C_2 &= -Bb_2 + b_2 y(x) + 2b_1 y'(x) + 2y''(x),\\ C_3 &= -Bb_3 + b_3 y(x) + 2b_2 y'(x) + 2b_1 y''(x) + \frac{4}{3} y'''(x),\\ C_4 &= 2b_3 y'(x) + 2b_2 y''(x) + \frac{4}{3} b_1 y'''(x) + \frac{2}{3} y^{(4)}(x),\\ C_5 &= 2b_3 y''(x) + \frac{4}{3} b_2 y'''(x) + \frac{2}{3} b_1 y^{(4)}(x) + \frac{4}{15} y^{(5)}(x)\}.\end{aligned}$$

With $C_0 = C_1 = C_2 = C_3 = C_4 = 0$, we obtain a system of five simultaneous equations which has the following solutions

$$\begin{Bmatrix} B = y(x), A = 2y'(x), b_1 = -\dfrac{y''(x)}{y'(x)}, b_2 = \dfrac{3y''(x)^2 - 2y'(x)y'''(x)}{3y'(x)^2}, \\ b_3 = \dfrac{-3y''(x)^3 + 4y'(x)y''(x)y'''(x) - y'(x)^2 y^{(4)}(x)}{3y'(x)^3} \end{Bmatrix}. \tag{25}$$

Substituting the parameters in (25) into C_5, we obtain

$$C_5 = -\frac{2\left(9y''(x)^4 - 18y'(x)y''(x)^2 y'''(x) + 4y'(x)^2 y'''(x)^2 + 6y'(x)^2 y''(x) y^{(4)}(x)\right)}{9y'(x)^3} + \frac{4}{15} y^{(5)}(x). \tag{26}$$

When $y(x)$ is now taken as the theoretical solution of the initial value problem (1) at a point x_n i.e. $y(x) = y(x_n)$, (25) can be written as

$$\left\{B = y_n, A = 2y'_n, b_1 = -\frac{y''_n}{y'_n}, b_2 = \frac{3(y''_n)^2 - 2y'_n y'''_n}{3(y'_n)^2}, b_3 = \frac{-3(y''_n)^3 + 4y'_n y''_n y'''_n - (y'_n)^2 y_n^{(4)}}{3(y'_n)^3}\right\}, \tag{27}$$

where $y_n = y(x_n)$ and $y_n^{(m)} = y^{(m)}(x_n)$, $m = 1,2,3,4$ by the localizing assumption. By taking $K = 3$, (2) becomes

$$y_{n+2} = B + \frac{Ah}{1 + b_1 h + b_2 h^2 + b_3 h^3}, \quad 1 + b_1 h + b_2 h^2 + b_3 h^3 \neq 0. \tag{28}$$

We indicate (28) based on (27) as RMM3(2,4), expressed in the form of

$$\begin{aligned} y_{n+2} = y_n + \left(6h(y_n')^4\right) \Big/ \Big(&3(y_n')^3 - 3h(y_n')^2 y_n'' + 3h^2 y_n' (y_n'')^2 - 3h^3 (y_n'')^3 \\ &-2h^2 (y_n')^2 y_n''' + 4h^3 y_n' y_n'' y_n''' - h^3 (y_n')^2 y_n^{(4)}\Big). \end{aligned} \tag{29}$$

From Definition 2 and (26), LTE of RMM3(2,4) is given by

$$\begin{aligned} &\mathrm{LTE}_{\mathrm{RMM3(2,4)}} \\ &= h^5 \left(-\frac{2\left(9(y_n'')^4 - 18 y_n' (y_n'')^2 y_n''' + 4(y_n')^2 (y_n''')^2 + 6(y_n')^2 y_n'' y_n^{(4)}\right)}{9(y_n')^3} \right. \\ &\qquad \left. + \frac{4}{15} y_n^{(5)} \right) + O\left(h^6\right), \end{aligned} \tag{30}$$

where $y_n^{(m)} = y^{(m)}(x_n)$, $m = 1,2,3,4,5$ by the localizing assumption.

If we apply RMM3(2,4) to the Dahlquist's test equation $y' = \lambda y$, $\mathrm{Re}(\lambda) < 0$, we obtain the following difference equation

$$y_{n+2} = \frac{3 + 3h\lambda + h^2\lambda^2}{3 - 3h\lambda + h^2\lambda^2} y_n. \tag{31}$$

Setting $z = h\lambda$, $y_{n+2} = \xi^2$ and $y_n = \xi^0 = 1$ in (31), we obtain the following characteristic equation

$$\xi^2 - \frac{3 + 3z + z^2}{3 - 3z + z^2} = 0. \tag{32}$$

The roots of (32) are

$$\xi_{(32,1)} = -\frac{\sqrt{3+3z+z^2}}{\sqrt{3-3z+z^2}} \text{ and } \xi_{(32,2)} = \frac{\sqrt{3+3z+z^2}}{\sqrt{3-3z+z^2}}.$$

By taking $z = x + \mathrm{i}y$ in the roots of (32), the region of absolute stability of RMM3(2,4) is exactly the one shown in Figure 1. We note that the characteristic equation of RMM3(2,3) given by (23) is identical to the characteristic equation of RMM3(2,4) shown in (32). The shaded region in Figure 1 becomes the region of absolute stability of RMM3(2,4), where the conditions: $\left|\xi_{(32,1)}\right| \le 1$ and $\left|\xi_{(32,2)}\right| \le 1$ are satisfied. Therefore it is obvious that RMM3(2,4) is *A*-stable.

6. 2-STEP FIFTH ORDER RMM3

In order to derive a fifth order RMM3, we have to take $K = 4$ in (3), expand $y(x+2h)$ into series to obtain following expression

$$\begin{aligned}
&L\left[y(x);h\right]_{\text{RMM3}} \\
&= -B + y(x) + h\left(-A - Bb_1 + b_1 y(x) + 2y'(x)\right) \\
&\quad + h^2\left(-Bb_2 + b_2 y(x) + 2b_1 y'(x) + 2y''(x)\right) \\
&\quad + h^3\left(-Bb_3 + b_3 y(x) + 2b_2 y'(x) + 2b_1 y''(x) + \frac{4}{3} y'''(x)\right) \\
&\quad + h^4\left(-Bb_4 + b_4 y(x) + 2b_3 y'(x) + 2b_2 y''(x) + \frac{4}{3} b_1 y'''(x) + \frac{2}{3} y^{(4)}(x)\right) \\
&\quad + h^5\left(2b_4 y'(x) + 2b_3 y''(x) + \frac{4}{3} b_2 y'''(x) + \frac{2}{3} b_1 y^{(4)}(x) + \frac{4}{15} y^{(5)}(x)\right) \\
&\quad + h^6\left(2b_4 y''(x) + \frac{4}{3} b_3 y'''(x) + \frac{2}{3} b_2 y^{(4)}(x) + \frac{4}{15} b_1 y^{(5)}(x) + \frac{4}{45} y^{(6)}(x)\right) + O\left(h^7\right).
\end{aligned} \tag{33}$$

Following Definition 1 and (4), it is readily deduced that

$$\{C_0 = -B + y(x), C_1 = -A - Bb_1 + b_1 y(x) + 2y'(x),$$
$$C_2 = -Bb_2 + b_2 y(x) + 2b_1 y'(x) + 2y''(x),$$
$$C_3 = -Bb_3 + b_3 y(x) + 2b_2 y'(x) + 2b_1 y''(x) + \frac{4}{3} y'''(x),$$
$$C_4 = -Bb_4 + b_4 y(x) + 2b_3 y'(x) + 2b_2 y''(x) + \frac{4}{3} b_1 y'''(x) + \frac{2}{3} y^{(4)}(x),$$
$$C_5 = 2b_4 y'(x) + 2b_3 y''(x) + \frac{4}{3} b_2 y'''(x) + \frac{2}{3} b_1 y^{(4)}(x) + \frac{4}{15} y^{(5)}(x),$$
$$C_6 = 2b_4 y''(x) + \frac{4}{3} b_3 y'''(x) + \frac{2}{3} b_2 y^{(4)}(x) + \frac{4}{15} b_1 y^{(5)}(x) + \frac{4}{45} y^{(6)}(x)\}.$$

With $C_0 = C_1 = C_2 = C_3 = C_4 = C_5 = 0$, we obtain a system of six simultaneous equations which has the following solutions

$$\left\{ B = y(x), A = 2y'(x), b_1 = -\frac{y''(x)}{y'(x)}, b_2 = \frac{3y''(x)^2 - 2y'(x)y'''(x)}{3y'(x)^2}, \right.$$
$$b_3 = \frac{-3y''(x)^3 + 4y'(x)y''(x)y'''(x) - y'(x)^2 y^{(4)}(x)}{3y'(x)^3}, \tag{34}$$
$$\left. \begin{aligned} b_4 = \big(&45y''(x)^4 - 90y'(x)y''(x)^2 y'''(x) + 20y'(x)^2 y'''(x)^2 \\ &+30y'(x)^2 y''(x) y^{(4)}(x) - 6y'(x)^3 y^{(5)}(x)\big) \big/ 45y'(x)^4 \end{aligned} \right\}.$$

Substituting the parameters in (34) into C_6, we obtain

$$\begin{aligned} C_6 = \Big(&30y''(x)\big(y''(x)^2 - 2y'(x)y'''(x)\big)\big(3y''(x)^2 - 2y'(x)y'''(x)\big) \\ &+10y'(x)^2 y^{(4)}(x)\big(9y''(x)^2 - 4y'(x)y'''(x)\big) - 24y'(x)^3 y''(x) y^{(5)}(x)\Big) \Big/ \\ &\big(45y'(x)^4\big) + \frac{4}{45} y^{(6)}(x). \end{aligned} \tag{35}$$

When $y(x)$ is now taken as the theoretical solution of the initial value problem (1) at a point x_n i.e. $y(x)=y(x_n)$, (34) can be written as

$$\left\{ B = y_n, A = 2y_n', b_1 = -\frac{y_n''}{y_n'}, \right.$$
$$b_2 = \frac{3(y_n'')^2 - 2y_n' y_n'''}{3(y_n')^2}, b_3 = \frac{-3(y_n'')^3 + 4y_n' y_n'' y_n''' - (y_n')^2 y_n^{(4)}}{3(y_n')^3},$$
$$\left. b_4 = \frac{45(y_n'')^4 - 90y_n'(y_n'')^2 y_n''' + 20(y_n')^2(y_n''')^2 + 30(y_n')^2 y_n'' y_n^{(4)} - 6(y_n')^3 y_n^{(5)}}{45(y_n')^4} \right\}, \tag{36}$$

where $y_n = y(x_n)$ and $y_n^{(m)} = y^{(m)}(x_n)$, $m = 1,2,3,4,5$ by the localizing assumption. By taking $K=4$, (2) becomes

$$y_{n+2} = B + \frac{Ah}{1 + b_1 h + b_2 h^2 + b_3 h^3 + b_4 h^4}, \quad 1 + b_1 h + b_2 h^2 + b_3 h^3 + b_4 h^4 \neq 0. \tag{37}$$

We indicate (37) based on (36) as RMM3(2,5), expressed in the form of

$$\begin{aligned} y_{n+2} &= y_n + \left(90h(y_n')^5\right) \Big/ \Big(45(y_n')^4 - 45h(y_n')^3 y_n'' + 45h^2(y_n')^2(y_n'')^2 - 45h^3 y_n'(y_n'')^3 \\ &\quad + 45h^4(y_n'')^4 - 30h^2(y_n')^3 y_n''' + 60h^3(y_n')^2 y_n'' y_n''' \\ &\quad - 90h^4 y_n'(y_n'')^2 y_n''' + 20h^4(y_n')^2(y_n''')^2 - 15h^3(y_n')^3 y_n^{(4)} \\ &\quad + 30h^4(y_n')^2 y_n'' y_n^{(4)} - 6h^4(y_n')^3 y_n^{(5)}\Big). \end{aligned} \tag{38}$$

From Definition 2 and (35), LTE of RMM3(2,5) is given by

$$\begin{aligned} &\mathrm{LTE}_{\mathrm{RMM3(2,5)}} \\ &= h^6\Big(\Big(30y_n''\big((y_n'')^2 - 2y_n' y_n'''\big)\big(3(y_n'')^2 - 2y_n' y''' \big) + 10(y_n')^2 y_n^{(4)}\big(9(y_n'')^2 - 4y_n' y_n'''\big) \\ &\quad -24(y_n')^3 y_n'' y_n^{(5)}\Big) \Big/ 45(y_n')^4 + \frac{4}{45} y_n^{(6)}\Big) + O(h^7), \end{aligned} \tag{39}$$

where $y_n^{(m)} = y^{(m)}(x_n)$, $m = 1,2,3,4,5,6$ by the localizing assumption.

If we apply RMM3(2,5) to the Dahlquist's test equation $y' = \lambda y$, $\mathrm{Re}(\lambda) < 0$, we obtain the following difference equation

$$y_{n+2} = \frac{45 + 45h\lambda + 15h^2\lambda^2 - h^4\lambda^4}{45 - 45h\lambda + 15h^2\lambda^2 - h^4\lambda^4} y_n . \tag{40}$$

Setting $z = h\lambda$, $y_{n+2} = \xi^2$ and $y_n = \xi^0 = 1$ in (40), we obtain the following characteristic equation

$$\xi^2 - \frac{45 + 45z + 15z^2 - z^4}{45 - 45z + 15z^2 - z^4} = 0 . \tag{41}$$

The roots of (41) are

$$\xi_{(41,1)} = -\frac{\sqrt{45 + 45z + 15z^2 - z^4}}{\sqrt{45 - 45z + 15z^2 - z^4}} \text{ and } \xi_{(41,2)} = \frac{\sqrt{45 + 45z + 15z^2 - z^4}}{\sqrt{45 - 45z + 15z^2 - z^4}} .$$

By taking $z = x + \mathrm{i}y$ in the roots of (41), we have plotted the region of absolute stability of RMM3(2,5) in Figure 2.

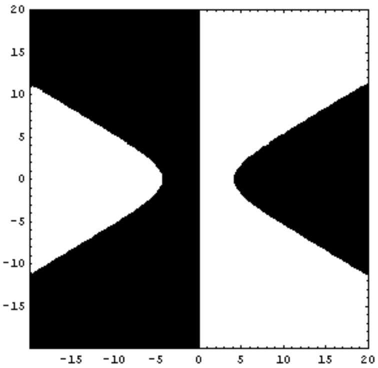

Figure 2: Stability region of RMM3(2,5).

The shaded region in Figure 2 is the region of absolute stability of RMM3(2,5), where the conditions: $\left|\xi_{(41,1)}\right| \le 1$ and $\left|\xi_{(41,2)}\right| \le 1$ are satisfied. From Figure 2, we can see that the region of absolute stability of

RMM3(2,5) does not contain the whole left-hand half plane which suggest that it is not *A*-stable.

7. NUMERICAL EXPERIMENTS AND COMPARISONS

In this section, some test problems are used to check the performance of all newly derived 2-step RMM3 using different number of integration steps. We present the maximum absolute errors over the integration interval given by $\max_{0\le n\le N}\left\{\left|y(x_n)-y_n\right|\right\}$ where N is the number of integration steps. We note that $y(x_n)$ and y_n are the exact solution and numerical solution of a test problem at point x_n , respectively. The numerical results obtained from our new proposed methods are compared with the numerical results obtained from the RMM2(2,*p*) of Teh *et al.* (2011) and the RMMs of Okosun and Ademiluyi (2007a), and Okosun and Ademiluyi (2007b). RMM2(2,*p*) can be easily identified from Teh *et al.* (2011). The following are those existing RMMs developed by Okosun and Ademiluyi (2007a), and Okosun and Ademiluyi (2007b): 2-step second order method given by

$$y_{n+2}=\frac{y_n^{\,3}}{y_n^{\,2}-2hy_ny_n'+h^2\left(4\left(y_n'\right)^2-2y_ny_n''\right)}, \tag{42}$$

3-step third order method given by

$$y_{n+3}$$
$$=\frac{2\left(y_n\right)^4}{2\left(y_n\right)^3-3h\left(y_n\right)^2\left(2y_n'+3h\left(y_n''+hy_n'''\right)\right)+18h^2y_ny_n'\left(y_n'+3hy_n''\right)-54h^3\left(y_n'\right)^3}, \tag{43}$$

4-step fourth order method given by

$$
\begin{aligned}
y_{n+4} = 3(y_n)^5 \Big/ \Big(& 3(y_n)^4 - 12h(y_n)^3 y_n' + h^2\left(48(y_n)^2(y_n')^2 - 24(y_n)^3 y_n''\right) \\
&+ h^3\left(192(y_n)^2 y_n' y_n'' - 192 y_n (y_n')^3 - 32(y_n)^3 y_n'''\right) \\
&+ h^4\Big(768(y_n')^4 - 1152 y_n (y_n')^2 y_n'' + 192(y_n)^2(y_n'')^2 \\
&\qquad + 256(y_n)^2 y_n' y_n''' - 32(y_n)^3 y_n^{(4)}\Big)\Big),
\end{aligned} \tag{44}
$$

and 5-step fifth order method given by

$$
\begin{aligned}
&y_{n+5} \\
&= 24(y_n)^6 \Big/ \Big(24(y_n)^5 - 120h(y_n)^4 y_n' - 300h^2(y_n)^3\left(y_n y_n'' - 2(y_n')^2\right) \\
&\qquad - 500h^3(y_n)^2\left(6(y_n')^3 - 6y_n y_n' y_n'' + (y_n)^2 y_n'''\right) \\
&\qquad - 625h^4 y_n\Big(36 y_n (y_n')^2 y_n'' - 24(y_n')^4 - 8(y_n)^2 y_n' y_n''' \\
&\qquad\qquad + (y_n)^2\left(y_n y_n^{(4)} - 6(y_n'')^2\right)\Big) \\
&\qquad - 625h^5\Big(120(y_n')^5 - 240 y_n (y_n')^3 y_n'' + 60(y_n)^2(y_n')^2 y_n''' \\
&\qquad\qquad - 10(y_n)^2 y_n'\left(y_n y_n^{(4)} - 9(y_n'')^2\right) + (y_n)^3\left(y_n y_n^{(5)} - 20 y_n'' y_n'''\right)\Big)\Big).
\end{aligned} \tag{45}
$$

The first step to implement the 2-step RMM3 (as well as 2-step RMM2) of order 2 until order 5, and RMMs in (42) – (45), is to choose a suitable method to calculate the value of y_1. It is desirable that y_1 should be calculated to an accuracy at least as high as the local accuracy of the RMMs (Lambert (1973)). Since RMM3(2,5) and RMMs in (45) possess the highest order of accuracy i.e. fifth order, then we choose the 6-stage fifth order Kutta-Nyström method showed on page 122 of Lambert (1973) to calculate the value of y_1 for 2-step RMM3 (as well as 2-step RMM2) of order 2 until order 5 and RMMs in (42) – (45).

The next step is to obtain the necessary higher derivatives of initial value problem in (1). To obtain the second order derivative y_n'', we just need to differentiate the initial value problem (1) once, that is

$$y''(x)\Big|_{x=x_n} = \left.\frac{df\left(x, y(x)\right)}{dx}\right|_{x=x_n} \approx y_n''.$$

Similarly, to obtain the third order derivative y_n''', we need to differentiate the initial value problem (1) twice, that is

$$y'''(x)\Big|_{x=x_n} = \left.\frac{d^2 f\left(x, y(x)\right)}{dx^2}\right|_{x=x_n} \approx y_n'''.$$

The fourth order and fifth order derivatives given by $y_n^{(4)}$ and $y_n^{(5)}$, respectively, can be easily obtain in this similar approach. On substituting the required derivatives into a particular RMM, then this RMM is ready to be used.

Problem 1 (Ramos (2007))

$$y'(x) = -100y(x) + 99e^{2x},\ y(0) = 0,\ x \in [0, 0.5].$$

The exact solution is given by $y(x) = \frac{33}{34}\left(e^{2x} - e^{-100x}\right)$. The maximum absolute errors for each method of different order are presented in Table 1 – Table 4.

Problem 2 (Yaakub and Evans (2003))

$$y''(x) + 101y'(x) + 100y(x) = 0,\ y(0) = 1.01,\ y'(0) = -2,\ x \in [0, 10].$$

The exact solution is given by $y(x) = 0.01e^{-100x} + e^{-x}$. *Problem 2* can also be written as a system, i.e.

$$y_1'(x) = y_2(x),\ y_1(0) = 1.01,\ x \in [0,10];$$
$$y_2'(x) = -100y_1(x) - 101y_2(x),\ y_2(0) = -2,\ x \in [0,10].$$

The exact solutions of this system are given by $y_1(x) = y(x) = 0.01e^{-100x} + e^{-x}$, $y_2(x) = y'(x) = -e^{-100x} - e^{-x}$. The maximum absolute errors for each method of different order are presented in Table 5 – Table 8.

Problem 3 (Ramos (2007))

$$y'(x) = 1 + y(x)^2,\ y(0) = 1,\ x \in [0,0.8].$$

Problem 3 is a problem whose solution possesses singularity. The exact solution is $y(x) = \tan(x + \pi/4)$. From the exact solution, we have noticed that the solution becomes unbounded in the neighbourhood of the singularity at $x = \pi/4 \approx 0.785398163367448$. The maximum absolute errors for each method of different order are presented in Table 9 – Table 12.

TABLE 1: Maximum Absolute Errors for Various Second Order Methods with respect to Number of Steps (*Problem 1*)

N	**RMM in (42)**	**RMM2(2,2)**	**RMM3(2,2)**
64	-	7.81545(-02)	7.81545(-02)
128	-	1.78169(-02)	1.78169(-02)
256	-	4.14749(-03)	4.14749(-03)
512	-	1.03195(-03)	1.03195(-03)

TABLE 2: Maximum Absolute Errors for Various Third Order Methods with respect to Number of Steps (*Problem 1*)

N	**RMM in (43)**	**RMM2(2,3)**	**RMM3(2,3)**
64	-	2.97028(-02)	5.85265(-03)
128	-	2.95546(-03)	6.14396(-04)
256	-	3.28246(-04)	7.41153(-05)
512	-	3.91259(-05)	9.17512(-06)

TABLE 3: Maximum Absolute Errors for Various Fourth Order Methods with respect to Number of Steps (*Problem 1*)

N	**RMM in (44)**	**RMM2(2,4)**	**RMM3(2,4)**
64	-	3.39927(-03)	3.31737(-03)
128	-	2.13926(-04)	2.03507(-04)
256	-	2.16793(-05)	1.29112(-05)
512	-	2.35624(-06)	8.11981(-07)

TABLE 4: Maximum Absolute Errors for Various Fifth Order Methods with respect to Number of Steps (*Problem 1*)

N	**RMM in (45)**	**RMM2(2,5)**	**RMM3(2,5)**
64	-	5.93616(-04)	3.16484(-04)
128	-	1.64123(-05)	9.19695(-06)
256	-	4.76120(-07)	2.94052(-07)
512	-	1.45048(-08)	9.35850(-09)

Table 1 – Table 4 have showed that existing RMMs in (42) – (45) cannot solve *Problem 1* with initial value equals to zero, but RMM2 of Teh *et al.* (2011) and RMM3 do not face such difficulty. From Table 2 and Table 4, we can see that the third order and fifth order 2-step RMM3 are more accurate than the third order and fifth order 2-step RMM2. However, results from Table 3 showed that both fourth order 2-step RMM2 and 2-step RMM3 are found to have comparable accuracy except for $N = 512$.

TABLE 5: Maximum Absolute Errors for Various Second Order Methods with respect to Number of Steps (*Problem 2*)

N	**RMM in (42)**	**RMM2(2,2)**	**RMM3(2,2)**
2560	1.20431(-03)	8.25702(-04)	8.25702(-04)
5120	2.88964(-04)	2.19023(-04)	2.19023(-04)
10240	7.04627(-05)	5.63484(-05)	5.63484(-05)

TABLE 6: Maximum Absolute Errors for Various Third Order Methods with respect to Number of Steps (*Problem 2*)

N	**RMM in (43)**	**RMM2(2,3)**	**RMM3(2,3)**
2560	2.59963(-03)	1.18777(-03)	1.21408(-03)
5120	6.90425(-04)	3.33834(-04)	3.36962(-04)
10240	1.79972(-04)	8.86875(-05)	8.90599(-05)

TABLE 7: Maximum Absolute Errors for Various Fourth Order Methods with respect to Number of Steps (*Problem 2*)

N	**RMM in (44)**	**RMM2(2,4)**	**RMM3(2,4)**
2560	2.43180(-03)	1.19841(-03)	1.19380(-03)
5120	8.32097(-04)	3.34438(-04)	3.34102(-04)
10240	2.42351(-04)	8.87017(-05)	8.86790(-05)

TABLE 8: Maximum Absolute Errors for Various Fifth Order Methods with respect to Number of Steps (*Problem 2*)

N	**RMM in (45)**	**RMM2(2,5)**	**RMM3(2,5)**
2560	3.30441(-03)	1.18719(-03)	1.18609(-03)
5120	1.05235(-03)	3.33575(-04)	3.33545(-04)
10240	3.11077(-04)	8.86222(-05)	8.86403(-05)

From Table 5, existing second order RMM in (42), RMM2(2,2) and RMM3(2,2) are found to have comparable accuracy except for $N = 2560$. Results from Table 6 showed that existing third order RMM in (43), RMM2(2,3) and RMM3(2,3) have comparable accuracy for $N = 2560$ and $N = 5120$, but not for $N = 10240$. For $N = 10240$, only RMM2(2,3) and RMM3(2,3) have comparable accuracy, and they are more accurate than the RMM in (43). The same pattern from Table 6 also emerges in Table 7. From Table 8, the fifth order RMM2(2,5) and RMM3(2,5) are more accurate than the existing RMM in (45) for $N = 5120$ and $N = 10240$. However, both RMM2(2,5) and RMM3(2,5) are found to have comparable accuracy for any number of integration steps.

TABLE 9: Maximum Absolute Errors for Various Second Order Methods with respect to Number of Steps (*Problem 3*)

N	**RMM in (42)**	**RMM2(2,2)**	**RMM3(2,2)**
64	7.85505(+01)	3.95730(+01)	3.95730(+01)
128	1.78097(+01)	9.46824(+00)	9.46824(+00)
256	1.74431(+01)	9.62127(+00)	9.62127(+00)
512	1.61376(+01)	8.81944(+00)	8.81944(+00)

TABLE 10: Maximum Absolute Errors for Various Third Order Methods with respect to Number of Steps (*Problem 3*)

N	**RMM in (43)**	**RMM2(2,3)**	**RMM3(2,3)**
64	4.96315(+00)	1.35285(-01)	1.52254(-03)
128	5.99106(-01)	1.72803(-02)	9.67085(-05)
256	3.01238(-01)	8.96655(-03)	2.53049(-05)
512	1.35801(-01)	4.03688(-03)	5.71518(-06)

TABLE 11: Maximum Absolute Errors for Various Fourth Order Methods with respect to Number of Steps (*Problem 3*)

N	**RMM in (44)**	**RMM2(2,4)**	**RMM3(2,4)**
64	5.86819(-01)	1.52254(-03)	1.52254(-03)
128	3.89199(-02)	9.67086(-05)	9.67085(-05)
256	1.00813(-02)	2.53043(-05)	2.53048(-05)
512	2.28366(-03)	5.71485(-06)	5.71529(-06)

TABLE 12: Maximum Absolute Errors for Various Fifth Order Methods with respect to Number of Steps (*Problem 3*)

N	**RMM in (45)**	**RMM2(2,5)**	**RMM3(2,5)**
64	9.07345(-02)	3.68169(-05)	1.97451(-08)
128	3.12186(-03)	1.40410(-06)	1.45553(-09)
256	3.97995(-04)	1.95575(-07)	4.97948(-10)
512	4.31393(-05)	3.14233(-08)	2.69665(-10)

From Table 9, second order RMM2(2,2) and RMM3(2,2) are more accurate than the existing RMM in (42), except for $N = 64$, where all three RMMs are found to have comparable accuracy. From Table 10, we can see that RMM3(2,3) generated the most accurate numerical results in solving *Problem 3*, followed by RMM2(2,3), and lastly, the existing RMM in (43). From Table 11, fourth order RMM2(2,4) and RMM3(2,4) are more accurate than the existing RMM in (44). Results from Table 12 have showed that RMM3(2,5) is the most accurate fifth order method compared to the existing RMM2(2,5) and RMM in (45).

From the numerical results shown in Table 1 – Table 9, we can summarize that RMM3(2,3) and RMM3(2,5) outperform RMM2(2,3), RMM2(2,5), RMM in (43) and RMM in (45) when solving initial value problem with single ordinary differential equation such as *Problem 1* and *Problem 3*. When solving initial value problem with coupled ordinary differential equations, all RMM3(2,*p*) and RMM2(2,*p*) have comparable accuracy. Therefore, the strength of RMM3(2,*p*) becomes apparent when solving initial value problem with single differential equation.

8. GENERALIZATIONS TO *r*-STEP *p*-TH ORDER RMM3

In the previous sections, we have showed the existence of some 2-step *p*-th order RMM3. Therefore it is reasonable to deduce that 2-step *p*-th order RMM3 can be generalized to *r*-step *p*-th order RMM3. From (2), we generalize 2-step RMM3 to *r*-step RMM3 given by

$$y_{n+r} = B + \frac{Ah}{1+\sum_{j=1}^{K} b_j h^j}, \quad 1+\sum_{j=1}^{K} b_j h^j \neq 0. \tag{46}$$

With the r-step RMM3 in (46), we associate the difference operator L defined by

$$L\left[y(x);h\right]_{\text{RMM3}} = \left(y(x+rh)-B\right)\times\left(1+\sum_{j=1}^{K} b_j h^j\right) - Ah, \tag{47}$$

where $y(x)$ is an arbitrary function, continuously differentiable on $x\in\left[a,b\right]\subset \mathrm{R}$. Expanding $y(x+rh)$ as Taylor series and collecting terms in (47) give the following expression:

$$L\left[y(x);h\right]_{\text{RMM3}} = C_0 h^0 + C_1 h^1 + \cdots + C_K h^K + C_{K+1} h^{K+1} + \cdots. \tag{48}$$

We note that C_i , $i = 0,1,\ldots,K,K+1,\ldots$ in (48) contain corresponding parameters which need to be determined in the derivation processes. Therefore, the order and local truncation error of r-step p-th order RMM3 based on (46) are defined as follows.

Definition 3. The difference operator (47) and the associated rational multistep method (46) are said to be of order $p = K+1$ if, in (48), $C_0 = C_1 = \cdots = C_{K+1} = 0$, $C_{K+2} \neq 0$.

Definition 4. The local truncation error at x_{n+r} of (46) is defined to be the expression $L\left[y(x_n);h\right]_{\text{RMM3}}$ given by (47), when $y(x_n)$ is the theoretical solution of the initial value problem (1) at a point x_n. The local truncation error of (46) is then

$$L\left[y(x_n);h\right]_{\text{RMM3}} = C_{K+2} h^{K+2} + O\left(h^{K+3}\right). \tag{49}$$

From Definition 3 and Definition 4, we have noticed that the order of accuracy of a r-step RMM3 is not affected by the number of step r.

Lastly, Table 13 shows those r-step RMM3 which have more values in computational practice, and can be considered in future studies.

TABLE 13: Potential r-step RMM3 of Order p.

p \ r	2	3	4	5	6	⋯⋯
2	√					
3	√	√				
4	√	√	√			
5	√	√	√	√		
6	√	√	√	√	√	
7	√	√	√	√	√	⋯⋯
⋮	⋮	⋮	⋮	⋮	⋮	⋱

9. CONCLUSION

In this article, we have presented the developments and applications of a new class of 2-step p-th order RMMs known to be RMM3(2,p). The general formulation of RMM3(2,p) is given in equation (2) while the order condition and local truncation error of RMM3 based on equation (2) are explained in Definition 1 and Definition 2. Absolute stability analysis showed that RMM3(2,2), RMM3(2,3) and RMM3(2,4) are A-stable, which make them suitable to solve stiff problems.

We have chosen three test problems to evaluate the effectiveness of RMM3(2,p) and other existing RMMs in terms of numerical accuracy. Most of the time, RMM3(2,3) and RMM3(2,5) generated more accurate numerical results compared to existing RMMs in solving initial value problem with single ordinary differential equation (such as *Problem 1* and *Problem 3*). However, RMM3(2,p) did not outperform the existing RMM2(2,p) when solving initial value problem with coupled ordinary differential equations (such as *Problem 2*). From these numerical experimentations, we can say that RMM3(2,p) is more reliable in solving problem with single ordinary differential equation.

Finally, we have showed that 2-step p-th order RMM3 can be generalized to r-step p-th order RMM3. The general formulation of a r-step p-th order RMM3 is given in equation (46) while the order condition and local truncation error of a r-step p-th order RMM3 are explained in Definition 3 and Definition 4. Future studies should discuss the properties of convergence, consistency, zero-stability and absolute stability of r-step p-th order RMM3. The generalization of the parameters in r-step p-th order RMM3 also constitutes a good problem for future study.

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