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Numerical Solutions of First Order Initial-Value Problem with Singularities and Stiffness Properties by a Rational Scheme

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In this paper, a scheme for solving first order singular and stiff differential equations is proposed. The studied approaches, namely Modified Rational Method (MRM), are developed based on a rational function mentioned by an existing study and possess second and third order of accuracy. Some modifications is implemented in the derivation technique, where closest points of approximation are considered in the formula of the methods. The proposed methods are both A-stable and suitable in solving problems with stiffness properties. The methods are not self-starting, thus the application of a suitable method to calculate the starting value is required in implementing these formulas. The results computed by the methods are found to be comparable to the existing methods.

Keywords: explicit rational method; singular initial-value problem; stiff DE

I. INTRODUCTION

Studies on numerical approaches that are developed for solving initial value problems (IVPs) of the form

$$y' = f(x, y), \quad y(a) = y_0, \quad x \in [a, b],$$

where a and b are the initial and the end points of the interval of x respectively, usually came from the class of linear methods, such as Linear Multistep Methods and Runge-Kutta Methods. Some methods are specially formulated for specific problems; for instance, Backward Differentiation Formula (BDF) for solving stiff problems and Rational Method for solving problems with singularity.

The suitability of numerical approaches that are based on rational function, or better known as rational method in solving many types of problems has intrigued many researchers to study more on this topic. Some literature rational methods are such as (Lambert & Shaw, 1965; Niekerk, 1987; Niekerk, 1988; Ikhile, 2001) for one-step schemes, while (Luke *et al.*, 1975; Fatunla, 1982; Fatunla, 1986; Abelman & Eyre, 1990; Okosun & Ademiluyi, 2007a; 2007b) for multistep schemes. Some studies on this topic focus on developing A-stable rational schemes so that the methods are suitable in solving stiff problems, for instance; (Ramos, 2007; Ramos *et al.*, 2015; Ramos *et al.*, 2017; Teh *et al.*, 2011).

One of the recent studies on rational multistep methods are done by (Teh & Yaacob, 2013), namely RMM3 which have the form of

$$y_{n+2} = y_n + \frac{2h(y_n')^2}{y_n' - hy_n''}. \qquad (1)$$

From the formula, it is obvious that the distance between the approximation points is two steplengths, or $2h$. Motivated by the study, we aim to develop a class of rational methods that will lessen the gap of the selected points of approximation. In order to develop such methods, we implement some modifications in the derivation technique of the proposed methods.

In this paper, the similar rational function as in (Teh & Yaacob, 2013) is considered to derive the proposed rational methods and the A-stability feature of the methods is

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ensured to facilitate the comparisons between the methods studied and some existing methods. The development, order, stability and implementations of the methods will be discussed in this paper. The presented methods in this article are examined on different types of problem; singular and stiff IVPs and the results are compared to the existing methods.

II. FRAMEWORK OF MODIFIED RATIONAL METHODS (MRM)

By referring to (Teh and Yaacob, 2013), we suggest the approximation for $y(x_{n+2})$ denoted by y_{n+2} and is given by;

$$y_{n+2} = B + h\left[\frac{Ah}{\sum_{j=1}^{K} c_j h^j}\right], \quad (2)$$

where A is real constant, while B and $c_j, j = 1,2,\dots,K$ are parameters that may contain approximations of $y(x_{n+1})$ and higher derivatives of $y(x_{n+1})$.

With the formula above, we associate the linear difference operator;

$$L[y(x);h]_{MRM} = [y(x_{n+2}) - B] \times \left[\sum_{j=1}^{K} c_j h^j\right] - Ah$$
$$= [y(x_{n+1}+h) - B] \times \left[\sum_{j=1}^{K} c_j h^j\right] - Ah, \quad (3)$$

where $y(x_{n+1}+h)$ is chosen to represent $y(x_{n+2})$ in order to lessen the gap between the approximated point and the point which is considered for the approximation process by the formula of the method. Meanwhile, $y(x)$ is arbitrary and continuously differentiable on $x \in [a,b]$. Next is to expand $y(x_{n+1}+h)$ as Taylor series around x_{n+1} and collecting terms in the difference operator in (3), and we will obtain an expression that can be generally written as;

$$L[y(x);h]_{MRM} = C_0h^0 + C_1h^1 + \cdots + C_Kh^K + C_{K+1}h^{K+1} + \cdots. \quad (4)$$

Note that $C_i, i = 0,1,\dots,K,K+1$ in expression (4) contain the parameters that are to be determined throughout the derivation process. The order and the parameters can be determined by referring to the definition:

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

Meanwhile, The local truncation errors of MRM are determined based on the definition below;

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

$$L[y(x);h]_{MRM} = C_{K+2}h^{K+2} + O(h^{K+3}). \quad (5)$$

A. Second Order Modified Rational Method (MRM(2))

In order to have the second order of MRM, we consider $K = 1$ in (2) so we will have the rational function in the form of;

$$y_{n+2} = B + \frac{Ah}{1 + c_1h}, \text{where } 1 + c_1h \neq 0 \quad (6)$$

and its associated linear difference operator as;

$$L[y(x);h]_{MRM(2)} = [y(x_{n+1}+h) - B] \times (1 + c_1h) - Ah \quad (7)$$

Next, expanding $y(x_{n+1}+h)$ as Taylor series around x_{n+1} will give the expression;

$$\begin{aligned} L[y(x);h]_{MRM(2)} &= -B + y(x_{n+1}) \\ &+ h[-A - Bc_1 + c_1y(x_{n+1}) + y'(x_{n+1})] \\ &+ h^2\left[c_1y'(x_{n+1}) + \frac{1}{2}y''(x_{n+1})\right] \\ &+ h^3\left[\frac{1}{2}c_1y''(x_{n+1}) + \frac{1}{6}y'''(x_{n+1})\right] + O(h^4) \end{aligned} \quad (8)$$

From (8), we obtain;

$$\begin{aligned} C_0 &= -B + y(x_{n+1}) \\ C_1 &= -A - Bc_1 + c_1y(x_{n+1}) + y'(x_{n+1}) \\ C_2 &= c_1y'(x_{n+1}) + \frac{1}{2}y''(x_{n+1}) \\ C_3 &= \frac{1}{2}c_1y''(x_{n+1}) + \frac{1}{6}y'''(x_{n+1}) \end{aligned} \quad (9)$$

Since $K = 1$ and according to Definition 1, $C_0 = C_1 = C_2 = 0$ and $C_3 \neq 0$; and we take y_{n+1} as the approximation of the theoretical solution $y(x_{n+1})$, thus the parameters in (6) are determined and can be written as;

$$\begin{aligned} A &= y'_{n+1}, \\ B &= y_{n+1}, \\ c_1 &= -\frac{y''_{n+1}}{2y'_{n+1}}, \end{aligned} \tag{10}$$

where by the localizing assumption, $y_{n+1} = y(x_{n+1})$ and $y^m_{n+1} = y^m(x_{n+1}),\ m = 1,2.$

By substituting the obtained parameters in (10) in C_3, we have;

$$C_3 = -\frac{(y''_{n+1})^2}{4y'_{n+1}} + \frac{y'''_{n+1}}{6}. \tag{11}$$

Based on equation (6) and (10), we formulate MRM(2) and it can be written as;

$$y_{n+2} = y_{n+1} + \frac{2h(y'_{n+1})^2}{2y'_{n+1} - hy''_{n+1}}. \tag{12}$$

As we refer to Definition 2 and (11), we obtain the local truncation error for MRM(2):

$$LTE_{MRM(2)} = h^3\left[-\frac{(y''_{n+1})^2}{4y'_{n+1}} + \frac{y'''_{n+1}}{6}\right] + O(h^4), \tag{13}$$

where by the localizing assumption, $y^m_{n+1} = y^m(x_{n+1}),\ m = 1,2,3.$

B. Third Order Modified Rational Method (MRM(3))

To derive a third order MRM, we need to consider $K = 2$ in (2) so the rational approximation associated to this method is

$$y_{n+2} = B + \frac{Ah}{1 + c_1h + c_2h^2}, \quad \text{where } 1 + c_1h + c_2h^2 \neq 0 \tag{14}$$

and the associated linear difference operator is given as

$$\begin{aligned} L[y(x);h]_{MRM(2)} &= [y(x_{n+1}+h) - B] \\ &\quad \times (1 + c_1h + c_2h^2) - Ah \end{aligned} \tag{15}$$

Next, we expand $y(x_{n+1}+h)$ as Taylor series to have the expression;

$$\begin{aligned} L[y(x);h]_{MRM(2)} &= -B + y(x_{n+1}) \\ &+ h[-A - Bc_1 + c_1y(x_{n+1}) + y'(x_{n+1})] \\ &+ h^2\left[-Bc_2 + c_2y(x_{n+1}) + c_1y'(x_{n+1}) + \frac{1}{2}y''(x_{n+1})\right] \\ &+ h^3\left[c_2y'(x_{n+1}) + \frac{1}{2}c_1y''(x_{n+1}) + \frac{1}{6}y'''(x_{n+1})\right] \\ &+ h^4\left[\frac{1}{2}c_2y''(x_{n+1}) + \frac{1}{6}c_1y'''(x_{n+1}) + \frac{1}{24}y^{(4)}_{n+1}\right] \\ &+ O(h^5) \end{aligned} \tag{16}$$

From (16); we obtain;

$$\begin{aligned} C_0 &= -B + y(x_{n+1}) \\ C_1 &= -A - Bc_1 + c_1y(x_{n+1}) + y'(x_{n+1}) \\ C_2 &= -Bc_2 + c_2y(x_{n+1}) + c_1y'(x_{n+1}) + \frac{1}{2}(x_{n+1}) \\ C_3 &= c_2y'(x_{n+1}) + \frac{1}{2}c_1y''(x_{n+1}) + \frac{1}{6}y'''(x_{n+1}) \\ C_4 &= \frac{1}{2}c_2y''(x_{n+1}) + \frac{1}{6}c_1y'''(x_{n+1}) + \frac{1}{24}y^{(4)}_{n+1} \end{aligned} \tag{17}$$

Since $K = 2$ and by following Definition 1, we have $C_0 = C_1 = C_2 = C_3 = 0$ and $C_4 \neq 0$, taking y_{n+1} as the approximation of the theoretical solution $y(x_{n+1})$, thus the parameters in (14) are determined as;

$$\begin{aligned} A &= y'_{n+1}, \\ B &= y_{n+1}, \\ c_1 &= -\frac{y''_{n+1}}{2y'_{n+1}}, \\ c_2 &= \frac{3(y''_{n+1})^2 - 2y'_{n+1}y'''_{n+1}}{12(y'_{n+1})^2}, \end{aligned} \tag{18}$$

where by the localizing assumption, $y_{n+1} = y(x_{n+1})$ and $y^m_{n+1} = y^m(x_{n+1}),\ m = 1,2,3.$

By substituting the obtained parameters in (18) in C_4, we have;

$$C_4 = \frac{(y''_{n+1})^3}{8(y'_{n+1})^2} - \frac{y''_{n+1}y'''_{n+1}}{6y'_{n+1}} + \frac{1}{24}y^{(4)}_{n+1}. \qquad (19)$$

Based on equation (14) and (18) we formulate MRM(3) and it can be written as;

$$y_{n+2} = y_{n+1} + \frac{12h(y'_{n+1})^3}{\begin{bmatrix} 12(y'_{n+1})^2 - 6hy'_{n+1}y''_{n+1} \\ +3h^2(y''_{n+1})^2 - 2h^2y'_{n+1}y'''_{n+1} \end{bmatrix}}. \qquad (20)$$

Referring to Definition 2 and (20), we obtain the local truncation error for MRM(3).

$$LTE_{MRM(3)} = h^4\left[\frac{(y''_{n+1})^3}{8(y'_{n+1})^2} - \frac{y''_{n+1}y'''_{n+1}}{6y'_{n+1}} + \frac{1}{24}y^{(4)}_{n+1}\right] + O(h^4), \qquad (21)$$

where by the localizing assumption,
$y^m_{n+1} = y^m(x_{n+1}),\ m = 1,2,3,4.$

III. STABILITY REGIONS OF MRM

The stability of the proposed rational methods can be analysed by applying it the Dahlquist's test equation, $y' = \lambda y,\ \ Re(\lambda) < 0$.

The A-stability of the methods can be identified according to the definition below;

Definition 3. *A numerical method is said to be A-stable if its region of absolute stability contains the whole left-hand half-plane Re $h\lambda < 0$.*

A. Stability of MRM(2)

To find the stability region for MRM(2) in (12), the formula of the method is applied to the test equation, and it yields the difference equation;

$$y_{n+2} = y_{n+1} + \left[\frac{2+\lambda h}{2-\lambda h}\right]. \qquad (22)$$

Taking $z = h\lambda, y_{n+2} = \xi^2$, and $y_{n+1} = \xi^1$, simplifying it and the stability function and the root, ξ can be obtained as;

$$R(z)_{MRM(2)} = \xi = \left[\frac{2+z}{2-z}\right]. \qquad (23)$$

Taking $z = x + iy$ into (23), we have plotted the absolute stability region of MRM(2) as in Figure 1, with the condition $|R(z)_{MRM(2)}| \le 1$ is satisfied.

Since the plotted stability region of MRM(2) (refer to Figure 1) is unbounded and contains the whole left-hand half-plane, thus it can be concluded that the second-order method is A-stable.

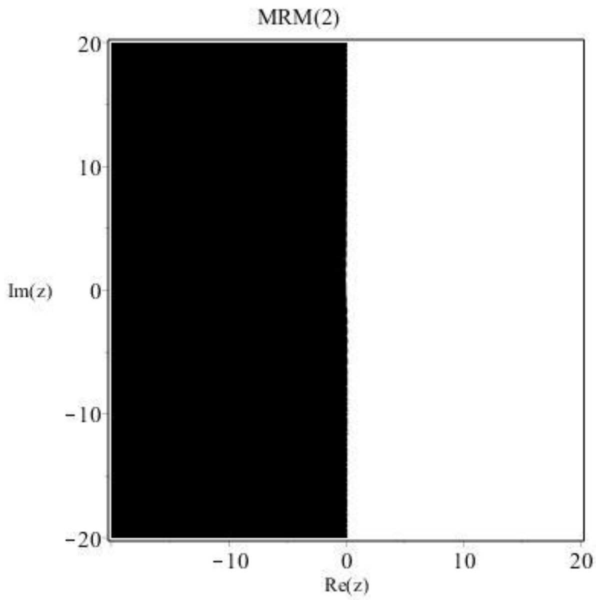

Figure 1. Absolute stability region of MRM(2)

B. Stability of MRM(3)

As MRM(3) in (20) is applied to the test equation, it gives the difference equation;

$$y_{n+2} = y_{n+1} + \left[\frac{12+6\lambda h+\lambda^2h^2}{12-6\lambda h+\lambda^2h^2}\right]. \qquad (24)$$

Taking $z = h\lambda, y_{n+2} = \xi^2$, and $y_{n+1} = \xi^1$, simplifying it and the stability function and the root, ξ can be obtained as;

$$R(z)_{MRM(3)} = \xi = \left[\frac{12+6z+z^2}{12-6z+z^2}\right]. \qquad (25)$$

Taking $z = x + iy$ into (25), we have plotted the absolute stability region of MRM(3) with the condition $|R(z)_{MRM(3)}| \le 1$ is satisfied and the region is found to be similar to the stability region of MRM(2), thus this method can also be concluded as A-stable.

IV. IMPLEMENTATION

The first step to implement the rational scheme developed in this study is to choose a suitable method to calculate the starting values as both methods are not self-starting. In this article, we apply the rational method of order four that is proposed by (Lambert, 1973) to compute the starting values. The formula of the method is given by;

$$y_{n+1} = y_n + hy_n' + \frac{h^2}{2}y_n'' + \frac{h^3}{6}y_n''' + \frac{h^4}{6}\left[\frac{y_n''' y_n^{(4)}}{4y_n''' - hy_n^{(4)}}\right] \quad (26)$$

Based on the formulation of the proposed rational methods; it is necessary to determine higher derivatives of the problem in order to compute the numerical solution. To obtain the higher derivatives of the IVP, differentiation of the equation of the problem is required;

$$y^{(k+1)}(x)\big|_{x=x_{n+1}} = \frac{df^k\big(x, y(x)\big)}{dx^k}\bigg|_{x=x_{n+1}} \approx y_{n+1}^{(k+1)}. \quad (27)$$

In this article, we compare the numerical results by MRM with several existing methods that have been introduced to solve singular and stiff problems. For comparison purposes we calculate the absolute error of each iteration given by;

$$(error_i)_n = \left|(y_i)_n - \big(y(x_i)\big)_n\right|. \quad (28)$$

The value of maximum and average of the absolute errors are considered for the comparison of accuracy of the methods in the study. In terms of efficiency, time of execution and total function evaluation are analysed.

V. NUMERICAL RESULTS AND DISCUSSION

In this section, several initial-value problems of different nature (singular and stiff) are tested using the proposed methods and compared with some of the existing methods.

(i) Problem 1 (Singular problem):
$y'(x) = 1 + y^2(x), \quad y(0) = 1, \quad 0 \le x \le 0.8$
Exact solution: $y(x) = \tan(x + \frac{\pi}{4})$
Singular point: $x = \frac{\pi}{4}$
Source: (Teh and Yaacob, 2013)

(ii) Problem 2 (Stiff problem):
$y'(x) = -100y(x) + 99e^{2x}, \quad y(0) = 1,$
$0 \le x \le 0.5$
Exact solution: $y(x) = \frac{33}{34}(e^{2x} - e^{-100x})$
Source: (Teh and Yaacob, 2013)

(iii) Problem 3 (Stiff problem):
$y'(x) = -10xy(x), \quad y(0) = 1, \quad 0 \le x \le 10$
Exact solution: $y(x) = e^{5x^2}$
Source: (Musa *et al.*, 2012)

The RMM3 of second and third order introduced by (Teh and Yaacob, 2013) is re-executed on the stated problems for comparison purposes in this article.

The tables below shows the numerical results for all the tested problems that have been solved using the proposed rational methods and are compared to several existing rational and BDF methods.

The notations used in the following tables are:

h	:	Step size
N	:	Number of subinterval
TF	:	Total function evaluation
AVE	:	Average error
MAX	:	Maximum error
Time	:	Time of execution in second
NS	:	Second Order Non-standard Method in (Ramos, 2007)
3BEBDF	:	3-Point Block Extended BDF in (Musa *et al.*, 2012)
2IBBDF	:	3-Point Improved Block BDF in (Musa *et al.*, 2013)
MRM(2)	:	Second Order Modified Rational Method proposed in this paper
MRM(3)	:	Third Order Modified Rational Method proposed in this paper
RMM(2,2)	:	2-step Second Order Rational Multistep Method in (Teh and Yaacob, 2013)
RMM(2,3)	:	2-step Third Order Rational Multistep Method in (Teh and Yaacob, 2013)
-	:	No data has been reported for this reference

Table 1 and 2 display the comparisons between MRM and existing rational methods of different order respectively. In Table 1, we can see that the performance of the MRM(2) are comparable to NS in terms of maximum and average error. Meanwhile, as MRM is compared to RMM3 of the same order in both tables, the proposed methods exhibit better accuracy and efficiency of approximation as its time of execution and total function function evaluation are smaller in value.

Table 3 and 4 portray the reliability of MRM in solving a stiff problems as compared to teh existing methods. It can be observed from the tables that MRM generates more accurate approximation compared NS and RMM3 of the same order based on displayed errors. Besides that, the execution time and total function evaluation of MRM is less than RMM3 indicating its efficiency in solving this problem.

In Table 5, MRM is compared to RMM3 as well as some BDF methods. From the table, we can see that the maximum errors and average errors given by MRM are

Table 1. Comparison Between MRM(2) and Second Order Rational Methods for Solving Problem 1

N	Methods applied	MAX	AVE	TF	Time
64	NS	9.47e+00	-	-	-
	RMM3(2,2)	3.96e+01	6.62e-01	132	7.90e-02
	MRM(2)	9.32e+00	1.57e-01	130	1.80e-02
128	NS	2.33e+00	-	-	-
	RMM3(2,2)	9.47e+00	1.04e-01	260	5.80e-02
	MRM(2)	2.31e+00	2.57e-02	258	5.20e-02
256	NS	2.43e+00	-	-	-
	RMM3(2,2)	9.62e+00	5.37e-02	516	4.98e-01
	MRM(2)	2.42e+00	1.35e-02	514	2.54e-01

Table 2. Comparison Between MRM(3) and RMM3(2,3) for Solving Problem 1

N	Methods applied	MAX	AVE	TF	Time
64	RMM3(2,3)	1.55e-03	2.61e-05	195	2.20e-02
	MRM(3)	1.22e-04	2.06e-06	193	1.90e-02
128	RMM3(2,3)	1.20e-04	1.33e-06	387	4.00e-02
	MRM(3)	2.93e-05	3.28e-07	385	1.69e-01
256	RMM3(2,3)	1.23e-04	6.84e-07	771	1.24e-01
	MRM(3)	9.96e-05	5.53e-07	769	1.22e-01

Table 3. Comparison Between MRM(2) and Second Order Rational Methods for Solving Problem 2

N	Methods applied	MAX	AVE	TF	Time
32	NS	1.78e-02	-	-	-
	RMM3(2,2)	7.82e-02	2.42e-03	68	3.00e-03
	MRM(2)	7.66e-03	3.21e-04	66	2.00e-03
64	NS	4.14e-03	-	-	-
	RMM3(2,2)	1.78e-02	6.51e-04	132	1.70e-02
	MRM(2)	2.70e-03	1.22e-04	130	1.60e-02
128	NS	1.03e-03	-	-	-
	RMM3(2,2)	4.15e-03	1.75e-04	260	4.90e-02
	MRM(2)	8.30e-04	3.79e-05	258	3.90e-02

Table 4. Comparison Between MRM(3) and RMM3(2,3) for Solving Problem 2

N	Methods applied	MAX	AVE	TF	Time
32	RMM3(2,3)	5.85e-03	3.52e-04	99	4.00e-03
	MRM(3)	4.20-04	3.26e-05	97	3.00e-03
64	RMM3(2,3)	6.14e-04	4.21e-05	195	2.70e-02
	MRM(3)	6.52e-05	4.44e-06	193	2.00e-02
128	RMM3(2,3)	7.41e-05	5.20e-06	387	9.40e-02
	MRM(3)	8.73e-06	6.01e-07	385	6.40e-02

smaller than the existing methods, which show that the proposed methods are capable in solving this problem. In terms of time of execution, MRM took shorter time to finish an execution compared to RMM3 of the same order.

VI. CONCLUSION

In this article, rational methods of second and third order are introduced where the closest points of approximation is taken into account in the derivation process. The proposed methods are found to be A-stable, which indicates that they are suitable in dealing with stiff equations. The numerical results presented in this research portray the capability of the proposed methods in solving IVPs with singularity and stiffness properties.

Table 5. Comparison Between MRM(2), MRM(3), RMM3 and Existing BDF Methods for Solving Problem 3

N	Methods applied	MAX	AVE	TF	Time
10^2	3BEBDF	-	-	-	-
	2IBBDF	-	-	-	-
	RMM3(2,2)	1.59e+00	2.70e-02	204	4.10e-02
	RMM3(2,3)	1.81e-01	6.15e-03	303	7.10e-02
	MRM(2)	4.25e-02	1.90e-03	202	3.90e-02
	MRM(3)	1.37e-02	7.25e-07	301	5.00e-02
10^3	3BEBDF	1.24e-02	-	-	-
	2IBBDF	1.50e-03	-	-	-
	RMM3(2,2)	2.00e+00	3.77e-02	2004	6.53e-01
	RMM3(2,3)	2.80e-03	1.03e-04	3003	7.64e-01
	MRM(2)	1.03e-03	4.85e-05	2002	4.22e-01
	MRM(3)	2.34e-04	9.41e-06	3001	4.68e-01
10^4	3BEBDF	7.36e-04	-	-	-
	2IBBDF	1.51e-05	-	-	-
	RMM3(2,2)	2.00e+00	3.94e-02	20004	5.06e+00
	RMM3(2,3)	3.00e-05	1.10e-06	30003	6.80e+00
	MRM(2)	1.57e-05	7.25e-07	20002	3.93e+00
	MRM(3)	2.53e-06	1.18e-07	30001	7.14e+00

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