# Rational Block Method for the Numerical Solution of First Order Initial Value Problem I: Concepts and Ideas

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### **Abstract**

In this study, the concept of block methods based on rational approximants is introduced for the numerical solution of first order initial value problems. These numerical methods are also called rational block methods. The main reason to consider rational block methods is to improve the numerical accuracy and absolute stability property of existing block methods that are based on polynomial approximants. For this pilot study, a 2-point explicit rational block method is developed. Local truncation error showed that the 2-point explicit rational block method possesses third order of accuracy. The absolute stability analysis showed that this new method has a finite region of absolute stability which shows that it is not A-stable. Several test problems are solved using the new method and three existing rational methods via constant step-size and variable step-size approaches. Numerical results generated by the 2-point explicit rational block method are promising in terms of numerical accuracy and computational cost. Finally, future issues on the developments of rational block methods are discussed.

### 1. INTRODUCTION

Numerical solutions for ordinary differential equations (ODEs) have great importance in scientific computation, as they are widely used to model the real world problems. Numerical solutions are desired to be as accurate as possible, which normally achieved by considering numerical methods with high order of consistency. However, computational cost would normally increase when numerical methods with greater order of consistency are applied. In view of this, there were many efforts being done in the past to reduce the computational cost but retain the desired accuracy. One of these many efforts being considered is the block methods. A block method can be considered as a set of simultaneously applied multistep methods to obtain several numerical approximations within each integration step [1]. Block methods are less expensive in terms of function evaluations of given order, and have the advantage of being self-starting [2]. While the issue of computational expenses is addressed, the stability requirements of block methods become more restricting when the order of consistency of the block methods increases, which make the numerical solution of stiff problem impossible for larger step-sizes. For excellence surveys and various perspectives of block methods, see, for example, Sommeijer et al. [1], Watanabe [3], Ibrahim et al. [4, 5], Chollom et al. [6], Majid et al. [7, 8], Mehrkanoon et al. [9], Akinfenwa et al. [10], Ehigie et al. [11], Ibijola et al. [12] and Majid and Suleiman [13].

Despite the shortcoming of block methods in terms of stability analysis, they are very useful tools in terms of solvability. Firstly, block methods can be easily modified and extended to solve higher order initial value problems directly, as reported in Majid et al. [7, 8], Ehigie et al. [11], Badmus and Yahaya [14] and Olabode [15]. Secondly, block methods can be easily implemented on a parallel machine, as reported in Sommeijer et al. [1], Mehrkanoon et al. [9] and Chartier [16]. Thus, the potential of block methods is obvious regardless of their stability drawbacks. In view of this, the research problem we are going to investigate is: "how can we develop block methods which possess strong stability requirements but cheaper computational costs?" Our readings have found out that there exist some unconventional numerical methods which possess strong stability conditions but yet explicit in nature. These unconventional methods are known as rational methods because they are numerical methods based on rational functions. Unfortunately, these explicit rational methods cannot generate several numerical approximations within each integration step like block methods. For excellence surveys and various perspectives of rational methods, see, for examples, Lambert [2], Lambert and Shaw [17], Luke et al. [18], Fatunla [19, 20], van Niekerk [21, 22], Ikhile [23, 24, 25], Ramos [26], Okosun and Ademiluyi [27, 28], Teh et al. [29, 30], Yaacob et al. [31], and Teh and Yaacob [32, 33]. By comparing the pros and cons of rational methods and block methods, we come out with the idea to search for block methods that are based on rational functions, or so called rational block methods (RBMs).

The main aim of this paper is to inroduce the concept and formulation idea of RBM through the development and implementation of a simple 2-point explicit RBM. The development of the said method is carried out in Section 2. After that, we demonstrate the calculation of principal local truncation error term and establish the absolute

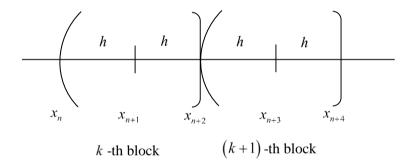
stability condition for the developed RBM in Section 3 and Section 4, respectively. In Section 5, the developed RBM and a few selected existing rational methods are tested in two settings: constant step-size, and variable step-size. Numerical comparisons are made and dicussed based on the numerical findings. Finally, some useful conclusions are drawn.

### 2. DERIVATION OF 2-POINT EXPLICIT BLOCK RATIONAL METHOD

The 2-point explicit rational block method, or in brief as 2-point ERBM, is formulated to solve the following first order initial value problem given by

$$y' = f(x, y), y(a) = \eta, \tag{1}$$

where  $f: \mathbb{R} \times \mathbb{R} \to \mathbb{R}$  and f(x,y) is assumed to satisfy all the required conditions such that problem (1) possesses a unique solution. Suppose that the interval of numerical integration is  $x \in [a,b] \subset \mathbb{R}$  and is divided into a series of blocks with each block containing two points as shown in Figure 1.



**Figure 1:** Two 2-point Consecutive Blocks.

From Figure 1, we observe that k-th block contains three points  $x_n$ ,  $x_{n+1}$  and  $x_{n+2}$ , and each of these points is separated equidistantly by a constant step-size h. The next (k+1)-th block also contains three points. In the k-th block, we want to use the values  $y_n$  at  $x_n$  to compute the approximation values of  $y_{n+1}$  and  $y_{n+2}$  simultaneously. In the (k+1)-th block, the previously computed value of  $y_{n+2}$  is used to generate the approximated values of  $y_{n+3}$  and  $y_{n+4}$ . The same computational procedure is repeated to compute the solutions for the next few blocks until the endpoint i.e. x = b is reached. The evaluation information from the previous step in a block can be used for other steps of the same block. The explanation provides here is nothing new and could be found in Majid et al. [8].

Along the x-axis, we consider the points  $x_n$ ,  $x_{n+1}$  and  $x_{n+2}$  to be given by  $x_n = x_0 + nh$ , (2)

$$x_{n+1} = x_0 + (n+1)h, (3)$$

and

$$x_{n+2} = x_0 + (n+2)h, (4)$$

where h is the step-size. Let us assume that the approximate solution of (1) is locally represented in the range  $[x_n, x_{n+1}]$  by the rational approximant

$$R(x) = \frac{a_0 + a_1 x + a_2 x^2}{b_0 + x},$$
(5)

where  $a_0$ ,  $a_1$ ,  $a_2$  and  $b_0$  are undetermined coefficients. This rational approximant in equation (5) is required to pass through the points  $(x_n, y_n)$  and  $(x_{n+1}, y_{n+1})$ , and moreover, must assume at these points the derivatives given by y' = f(x, y), y'' = f'(x, y) and y''' = f''(x, y). Altogether, there are five equations to be satisfied i.e.

$$R(x_n) = y_n, (6)$$

$$R(x_{n+1}) = y_{n+1}, (7)$$

$$R'(x_n) = y_n', (8)$$

$$R''(x_n) = y_n'', (9)$$

and

$$R'''(x_n) = y_n''', \tag{10}$$

where  $y'_n = f_n = f(x_n, y_n)$ ,  $y''_n = f'_n = f'(x_n, y_n)$  and  $y'''_n = f''_n = f''(x_n, y_n)$ . On using *MATHEMATICA 8.0*, the elimination of the four undetermined coefficients  $a_0$ ,  $a_1$ ,  $a_2$  and  $b_0$  from equations (6) – (10) yields the one-step rational method

$$y_{n+1} = y_n + hy_n' + \frac{h^2}{2} \frac{3(y_n'')^2}{3y_n'' - hy_n'''}.$$
 (11)

We note that equation (11) is exactly the one-step third order rational method proposed by Lambert and Shaw [17]. Equation (11) is the formula to approximate  $y_{n+1}$  by using the information at the previous point  $(x_n, y_n)$ .

To approximate  $y_{n+2}$ , we have to assume that the approximate solution of (1) is locally represented in the range  $[x_n, x_{n+2}]$  by the same rational approximant given in equation (5). It is crucial to retain the same rational approximant in the same block. Now, we required the rational approximant (5) to pass through the points  $(x_n, y_n)$ ,  $(x_{n+1}, y_{n+1})$  and  $(x_{n+2}, y_{n+2})$ , and moreover, must assume at these points the derivative

given by y' = f(x, y). There are also five equations to be satisfied i.e.

$$R(x_n) = y_n, (12)$$

$$R(x_{n+1}) = y_{n+1}, (13)$$

$$R(x_{n+2}) = y_{n+2},$$
 (14)

$$R'(x_n) = y_n', (15)$$

and

$$R'(x_{n+1}) = y'_{n+1}, (16)$$

where  $y'_n = f_n = f(x_n, y_n)$  and  $y'_{n+1} = f_{n+1} = f(x_{n+1}, y_{n+1})$ . On using *MATHEMATICA* 8.0, the elimination of the four undetermined coefficients  $a_0$ ,  $a_1$ ,  $a_2$  and  $b_0$  from equations (12) – (16) yields the following two-step rational method,

$$3y_{n+2} = 4y_{n+1} - y_n + \frac{2h}{3} (y'_n + 2y'_{n+1}) + \frac{4h^2}{3} \frac{(y'_n - y'_{n+1})^2}{3(y_{n+1} - y_n) - h(y'_{n+1} + 2y'_n)}.$$
 (17)

We note that equation (17) is exactly the two-step third order rational method proposed by Lambert and Shaw [17]. Equation (17) is the formula to approximate  $y_{n+2}$  by using the information at the previous points  $(x_n, y_n)$  and  $(x_{n+1}, y_{n+1})$ . Hence, the 2-point ERBM based on the rational approximant (5) consists of two formulae i.e. formulae (11) and (17).

The implementation of the 2-point ERBM is rather simple: with  $y_n$  is known, compute the approximate solution  $y_{n+1}$  using formula (11); and then compute the approximate solution  $y_{n+2}$  using formula (17) with the value of  $y_{n+1}$  obtained from formula (11).

# 3. LOCAL TRUNCATION ERRORS AND ORDER OF CONSISTENCY

To obtain the order of consistency of the 2-point ERBM, we would need to investigate the order of consistency of formulae (11) and (17) individually, which can be found by establishing the local truncation errors for both (11) and (17). Since formulae (11) and (17) are used in the same block to solve for the approximate solutions at  $x_{n+1}$  and  $x_{n+2}$ , we wish to have both formulae possess the same order of consistency. For formula (11), we can associate the following nonlinear operator defined by

$$L[y(x);h] = y(x+h) - y(x) - hy'(x) - \frac{h^2}{2} \frac{3y''(x)^2}{3y''(x) - hy'''(x)},$$
(18)

where y(x) is an arbitrary function, continuously differentiable on [a,b]. From

equation (18), on expanding y(x+h) in Taylor series about x, we obtain

$$L[y(x);h] = h^{4} \left(\frac{y^{(4)}(x)}{24} - \frac{y'''(x)^{2}}{18y''(x)}\right) + O(h^{5}).$$
(19)

Equation (19) indicates that formula (11) has third order of consistency, and the local truncation error (LTE) for formula (11) can be written as

LTE<sub>(11)</sub> = 
$$L[y(x_n); h] = h^4 \left( \frac{y_n^{(4)}}{24} - \frac{(y_n^{(3)})^2}{18y_n''} \right) + O(h^5),$$
 (20)

where y(x) is now taken to be the theoretical solution of problem (1).

For formula (17), the associate nonlinear operator is defined as follows

$$L[y(x);h] = 3y(x+2h) - 4y(x+h) + y(x) - \frac{2h}{3}(y'(x) + 2y'(x+h))$$

$$-\frac{4h^2}{3} \frac{(y'(x) - y'(x+h))^2}{3(y(x+h) - y(x)) - h(y'(x+h) + 2y'(x))},$$
(21)

where y(x) is an arbitrary function, continuously differentiable on [a,b]. From equation (21), on expanding y(x+h), y(x+2h) and y'(x+h) in Taylor series about x, we obtain

$$L[y(x);h] = h^{4} \left(\frac{y^{(4)}(x)}{2} - \frac{2}{3} \frac{y'''(x)^{2}}{y''(x)}\right) + O(h^{5}).$$
 (22)

Equation (22) indicates that formula (17) has third order of consistency, and the LTE for formula (17) can be written as

$$LTE_{(17)} = h^4 \left( \frac{y_n^{(4)}}{2} - \frac{2}{3} \frac{(y_n''')^2}{y_n''} \right) + O(h^5), \tag{23}$$

where y(x) is now taken to be the theoretical solution of problem (1).

From the local truncation errors given in equations (20) and (23), we can see that both formulae (11) and (17) possess third order of consistency. This also indicates that the 2-point ERBM is effectively of order 3.

# 4. ABSOLUTE STABILITY ANALYSIS

To investigate the linear stability condition for formulae (11) and (17) in the same block, we need to combine both formulae and apply the Dahquist's test equation

$$y' = \lambda y$$
,  $y(a) = y_0$ ,  $Re(\lambda) < 0$ ,

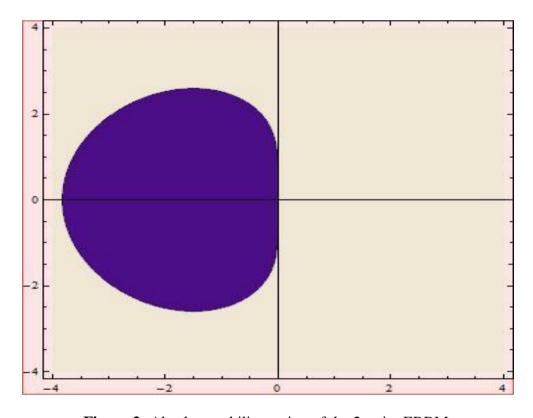
to both formulae. With  $y'_{n+1} = \lambda y_{n+1}$ ,  $y'_n = \lambda y_n$ ,  $y''_n = \lambda^2 y_n$ , and  $y'''_n = \lambda^3 y_n$ , we can obtain the following difference equation

$$y_{n+2} = \frac{9 + 12h\lambda + 7h^2\lambda^2 + 2h^3\lambda^3}{(h\lambda - 3)^2} y_n.$$
 (24)

On setting  $h\lambda = z$ ,  $y_{n+2} = \zeta^2$  and  $y_n = \zeta^0 = 1$  in equation (24), then the stability polynomial for the 2-point ERBM is

$$\zeta^{2} - \frac{9 + 12z + 7z^{2} + 2z^{3}}{(z - 3)^{2}} = 0.$$
 (25)

Here,  $\zeta$  can be interpreted as the roots of stability polynomial (25). By taking z = x + iy in the roots of equation (25), we have plotted the region of absolute stability of the 2-point ERBM in Figure 2.



**Figure 2:** Absolute stability region of the 2-point ERBM.

The shaded region in Figure 2 is the region of absolute stability of the 2-point ERBM. Hence, this shaded region can also be viewed as the 'combined' region of absolute stability of formulae (11) and (17). The shaded region is the place where the absolute

value of each root of equation (25) is less than or equal to 1. From Figure 2, we can see that the region of absolute stability does not contain the whole left-hand half plane which shows that the 2-point ERBM is not A-stable.

# 5. NUMERICAL EXPERIMENTS AND COMPARISONS

Through several test problems, the 2-point ERBM and a few selected existing rational methods are tested in two settings: constant step-size, and variable step-size. The constant step-size approach is pretty straightforward, where the interval of integration [a,b] is divided into a number of subintervals  $[x_n,x_{n+1}]$  of equal length h, and the numerical solutions at these nodal points are obtained by numerical methods. We first describe the variable step-size strategy for conventional one-step and multistep methods, and then we see how this strategy is suited for the 2-point ERBM.

# 5.1 Variable Step-size Algorithm for Conventional One-step or Multistep Methods

Suppose that we have solved numerically the initial value problem (1) using a k-step method, up to a point  $x_{n+k-1}$  and have obtained a value  $y_{n+k-1}$  as an approximation of  $y(x_{n+k-1})$ , which is the theoretical solution of problem (1). For every integration step, there is always a step-size, say  $h_s$  available to compute two approximations to the solution of problem (1), namely  ${}^{(s)}y_{n+k}$  and  ${}^{(s)}\hat{y}_{n+k}$  where s represents the (current) s-th iteration. First, the value  ${}^{(s)}y_{n+k}$  is obtained with step-size  $h_s$ . After that, integrate twice by halving the step-size  $h_s$  i.e.  $h_s/2$ , yields the value of  ${}^{(s)}\hat{y}_{n+k}$ . Then an estimate of the error for the less precise result is  $err = \left\| {}^{(s)}\hat{y}_{n+k} - {}^{(s)}y_{n+k} \right\|_{\infty}$ . We want this error estimation to satisfy

$$\left\| {^{(s)}}\hat{y}_{n+k} - {^{(s)}}y_{n+k} \right\|_{\infty} \le TOL, \tag{26}$$

where TOL is the desired tolerance prescribed by the user. If the inequality (26) is satisfied, then the computed step is accepted and this also means that  $^{(s)}y_{n+k}$  is accepted as  $y_{n+k}$ , and will be used to compute  $y_{n+k+1}$ . The current  $h_s$  is now used to advance to the next integration step to find  $y_{n+k+1}$ .

If the inequality (26) is not satisfied by the current  $h_s$ , i.e.

$$\| (s) \hat{y}_{n+k} - (s) y_{n+k} \|_{\infty} > TOL,$$
 (27)

then the computed value of  $^{(s)}y_{n+k}$  and the current  $h_s$  are rejected. Following this, we

need to start another iteration, say (s+1)-th iteration, with a new step-size, say  $h_{s+1}$ . The step-size  $h_{s+1}$  can be calculated as follows

$$h_{s+1} = h_s \times r \,, \tag{28}$$

where

$$r = \min\left(\max\left(0.5, 0.9 \left(\frac{TOL}{err}\right)^{\frac{1}{p+1}}\right), 1.0\right). \tag{29}$$

At this point,  $h_{s+1}$  is not used to advance to the next integration step, but remain in the current integration step to recalculate two approximate solutions, say  $^{(s+1)}y_{n+k}$  and  $^{(s+1)}\hat{y}_{n+k}$ . We note that  $^{(s+1)}y_{n+k}$  is obtained with step-size  $h_{s+1}$ . On integrating twice by halving the step-size  $h_{s+1}$  i.e.  $h_{s+1}/2$ , yields the value of  $^{(s+1)}\hat{y}_{n+k}$ . Then, the validation processes take place again using the inequalities

$$\| (s+1) \hat{y}_{n+k} - (s+1) y_{n+k} \|_{\infty} \le TOL$$
,

or

$$\left\| {^{(s+1)}}\hat{y}_{n+k} - {^{(s+1)}}y_{n+k} \right\|_{\infty} > TOL.$$

The iterating process to recalculate the current  $y_{n+k}$  is repeated, every time with a new adjusted step-size using equations (28) and (29) until the error estimation is less than the prescribed toleration.

Let's briefly explain equation (29). From equation (29), p is the order of the underlying k-step method, and  $\left(\frac{TOL}{err}\right)^{\frac{1}{p+1}}$  was multiplied by 0.9, where 0.9 is known as the safety factor. The safety factor was introduced to increase the possibility that the error will be accepted next time as the new step-size is also accepted [34, 35]. Furthermore, to prevent the new step-size from increasing or decreasing too fast, the step-size ratio was usually forced to lie between two bounds such as 0.5 and 1.0 [34, 35].

While applying the variable step-size strategy, there is another crucial element that we need to take good care of. Since step-size will be varied throughout the computation, there will be at one point where the step-size exceeded the right boundary of the integration interval [a,b]. In order to track this kind of situation, every time when a step-size  $h_s$  is calculated at any point of x, we must check whether  $x+h_s$  still lies in the interval [a,b] i.e.

$$x + h_{s} < b. ag{30}$$

If (30) is satisfied, then the computation continues without any interruption. However, if  $x + h_s$  is found to coincide with or greater than the right boundary b i.e.

$$x + h_{s} \ge b, \tag{31}$$

then the current step-size  $h_s$  is immediately rejected. The rejected current step-size  $h_s$  is then replaced by a final step-size, say  $h_b$  which can be obtained using the formula

$$h_b = b - x. (32)$$

Then, the last integration is performed to obtain the numerical approximation at the point x = b, say  $y_b$ , using the new step-size  $h_b$  obtained from (32).

# 5.2 Variable Step-size Algorithm for 2-point ERBM

The variable step-size algorithm for 2-point ERBM is very much resembles the variable step-size algorithm for conventional one-step and multistep methods presented in Section 5.1. Suppose that we have solved numerically the initial value problem (1) using the 2-point ERBM 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 problem (1).

For every integration step, there is always a step-size, say  $h_s$  available to compute two approximations to the solution of problem (1), namely  $^{(s)}y_{n+1}$  using formula (11) and  $^{(s)}y_{n+2}$  using formula (17) where s represents the (current) s-th iteration. After that, integrate twice by halving the step-size  $h_s$  i.e.  $h_s/2$ , yields the values of  $^{(s)}\hat{y}_{n+1}$  using formula (11) and  $^{(s)}\hat{y}_{n+2}$  using formula (17). Then an estimate of the error for the less precise result is  $err = \left\| {^{(s)}\hat{y}_{n+2} - {^{(s)}y_{n+2}}} \right\|_{\infty}$ . It is important to note that the estimate error is always performed on the approximate solution obtained by formula (17), not on the approximate solution obtain by formula (11). This error estimation is used to control the error of a block. We want this error estimation to satisfy

$$\left\| {^{(s)}}\hat{y}_{n+2} - {^{(s)}}y_{n+2} \right\|_{\infty} \le TOL, \tag{33}$$

where TOL is the desired tolerance prescribed by the user. If the inequality (33) is satisfied, then the computed step is accepted and this also means that  $^{(s)}y_{n+1}$  is accepted as  $y_{n+1}$  and  $^{(s)}y_{n+2}$  is accepted as  $y_{n+2}$ . The value  $y_{n+2}$  is then used to start the computation of the next block. The current  $h_s$  is now used to advance to the next block.

If the inequality (33) is not satisfied by the current  $h_s$ , i.e.

$$\| (s) \hat{y}_{n+2} - (s) y_{n+2} \|_{\infty} > TOL,$$
 (34)

then the computed values of  ${}^{(s)}y_{n+1}$ ,  ${}^{(s)}y_{n+2}$  and the current  $h_s$  are rejected. Following this, we need to start another iteration, say (s+1)-th iteration, with a new step-size, say  $h_{s+1}$ . The step-size  $h_{s+1}$  can be calculated using formulae (28) and (29). From equation (29), we note that p=3 is the order of the 2-point ERBM. At this point,  $h_{s+1}$ is not used to advance to the next block, but remain in the current block to obtain: (s+1) $y_{n+1}$  and (s+1) $y_{n+2}$  via the step-size  $h_{s+1}$ , and (s+1) $\hat{y}_{n+1}$  and (s+1) $\hat{y}_{n+2}$  by halving the step-size  $h_{s+1}$  i.e.  $h_{s+1}/2$ . Then, the validation processes take place again using the inequalities

$$\| (s+1) \hat{y}_{n+2} - (s+1) y_{n+2} \|_{\infty} \le TOL$$
,

or

$$\left\| {^{(s+1)}}\hat{y}_{n+2} - {^{(s+1)}}y_{n+2} \right\|_{\infty} > TOL.$$

The iterating process to recalculate the values of  $y_{n+1}$  and  $y_{n+2}$  in the current block is repeated, every time with a new adjusted step-size using equations (28) and (29) until the error estimation is less than the prescribed toleration.

To prevent the step-size from exceeding the right boundary of the integration interval [a,b], every time when a step-size  $h_s$  is calculated at any point of x, we must check whether  $x + 2h_s$  still lie in the interval [a,b] i.e.

$$x + 2h_s < b. (35)$$

If (35) is satisfied, then the computation continues without any interruption. However, if  $x + 2h_s$  is found to coincide with or greater than the right boundary b i.e.

$$x + 2h_{\rm s} \ge b \,, \tag{36}$$

then current step-size  $h_s$  is immediately rejected. The rejected current step-size  $h_s$  is then replaced by a final step-size, say  $h_b$  which can be obtained using the formula

$$h_b = \frac{b - x}{2} \,. \tag{37}$$

Then, the last integration is performed at the last block to obtain the last two numerical approximations using the new step-size  $h_b$  obtained from (37). We note that the  $h_s$  in equations (35) and (36) has to be multiplied by 2, whereas b-x has to be divided by 2 to obtain  $h_b$ . This is due to the nature of the 2-point ERBM for able to obtain two approximate solutions i.e. each approximate solution for a step-size  $h_s$ .

### 6. NUMERICAL TESTS AND RESULTS

In this section, we solved *Problem 1 – Problem 4* with the constant step-size approach and with the variable step-size strategy described in Section 5.2, using the 2-point ERBM (as in formulae (11) and (17)), and existing third order rational methods from van Niekerk [21], van Niekerk [22], and Ramos [26]. For the case of constant step-size, it is sufficient to present the maximum absolute relative errors over the integration interval [a,b] given by  $\max_{0 \le n \le N} \{|y(x_n) - y_n|\}$  where N is the number of subintervals. We note that  $y(x_n)$  and  $y_n$  represent the theoretical solution and numerical solution of a test problem at point  $x_n$ , respectively.

However, for the case of variable step-size, it is less informative if we only present the maximum absolute relative errors. It is because there are other parameters such as the tolerance Tol which will affect the total number of successful steps within the interval [a,b]. We denote:

- a. TOL as the user prescribed tolerance TOL,
- b. METHOD as the various third order rational methods used in comparison,
- c. SSTEP as the total number of successful steps within the interval [a,b],
- d. FSTEP as the total number of rejected steps with in the interval [a,b], and
- e. MAXE as the maximum absolute relative error defined by  $\max_{0 \le n \le \text{NSTEP}} \{ |y(x_n) y_n| \}$ .

### Problem 1

$$y'(x) = -2y(x) + 4x$$
,  $y(0) = 3$ ,  $x \in [0, 0.5]$ .

The theoretical solution is  $y(x) = 4e^{-2x} - 1 + 2x$ .

*Problem 2* [19]

$$y'(x) = -2000e^{-200x} + 9e^{-x} + xe^{-x}, y(0) = 10, x \in [0,1].$$

The theoretical solution is  $y(x) = 10 - 10e^{-x} - xe^{-x} + 10e^{-200x}$ .

*Problem 3* [5]

$$y'_1(x) = 198y_1(x) + 199y_2(x), y_1(0) = 1, x \in [0,10];$$
  
 $y'_2(x) = -398y_1(x) - 399y_2(x), y_2(0) = -1, x \in [0,10];$ 

The theoretical solutions are  $y_1(x) = e^{-x}$  and  $y_2(x) = -e^{-x}$ .

**Problem 4** [36]

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

The theoretical solution is  $y(x) = 0.01e^{-100x} + e^{-x}$ . Problem 4 can be reduced to a system of first order differential equations, 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 theoretical solutions are  $y_1(x) = 0.01e^{-100x} + e^{-x}$  and  $y_2(x) = -e^{-100x} - e^{-x}$ .

# **6.1 Constant Step-size Approach**

Table 1 until Table 5 showed the maximum absolute relative errors of various third order methods which obtained using the constant step-size.

**Table 1:** Maximum absolute relative errors of various third order methods (*Problem 1*)

$\overline{N}$	van Niekerk [21]	van Niekerk [22]	Ramos [26]	2-point ERBM
16	3.25864(-04)	5.07503(-06)	5.84945(-05)	8.09971(-07)
32	2.93414(-05)	6.28976(-07)	7.85013(-06)	5.17853(-08)
64	3.83339(-06)	7.82908(-08)	1.01742(-06)	3.27370(-09)

**Table 2:** Maximum absolute relative errors of various third order methods (*Problem 2*)

		(- : )		
$\overline{N}$	van Niekerk [21]	van Niekerk [22]	Ramos [26]	2-point ERBM
10	1.51502(+00)	7.08987(+01)	4.71235(+00)	7.73073(+01)
100	3.57558(-01)	7.48249(-01)	6.24419(-02)	6.46710(-01)
1000	1.44188(-03)	1.06282(-03)	1.34363(-03)	1.92485(-04)
10000	1.89317(-06)	1.10728(-06)	1.44295(-05)	2.19011(-08)

**Table 3:** Maximum absolute relative errors of various third order methods  $(y_1(x))$ 

(Frotiem 3)					
$\overline{N}$	van Niekerk [21]	van Niekerk [22]	Ramos [26]	2-point ERBM	
160	1.71953(-01)	2.39414(+82)	1.70066(-01)	2.02493(-07)	
320	1.11802(+03)	2.83659(+06)	1.24639(-02)	1.29463(-08)	
640	1.27418(-04)	2.00390(-04)	7.47140(-03)	8.18426(-10)	

Table 4: Maximum absolute relative errors of various third order methods	$(y_2(x))$	

$\overline{N}$	van Niekerk [21]	van Niekerk [22]	Ramos [26]	2-point ERBM
160	1.82388(-01)	4.78828(+82)	1.74387(-01)	2.02493(-07)
320	1.70960(+03)	5.67318(+06)	1.81547(-02)	1.29463(-08)
640	1.27417(-04)	2.00920(-04)	7.51943(-03)	8.18426(-10)

**Table 5:** Maximum absolute relative errors of various third order methods (*Problem 4*)

		(2 : 0010:11 1	,	
N	van Niekerk [21]	van Niekerk [22]	Ramos [26]	2-point ERBM
1280	1.67276(-04)	2.91323(-05)	2.15408(-05)	4.06612(-05)
2560	1.56050(-05)	3.12721(-06)	3.18139(-06)	2.35650(-06)
5120	1.24983(-06)	3.67925(-07)	4.38761(-07)	1.68714(-07)

Results from Table 1 until Table 5 indicate that 2-point ERBM is able to generate converging approximate solutions as the number of integration steps increases. 2-point ERBM is stable in solving very stiff problem such as *Problem 2*, and mildly stiff problems such as *Problem 3* and *Problem 4*, as observed from Table 2 until Table 5. The 2-point ERBM is also seem to be more accurate in solving *Problem 1*, *Problem 2* and *Problem 3*; and found to have comparable accuracy with the existing methods in solving *Problem 4*.

In short, for constant step-size approach, N also represents the number of integration steps, which is true for the existing third order rational methods of van Niekerk [21], van Niekerk [22] and Ramos [26]. As for the 2-point ERBM, the number of integration steps is actually N/2. Hence, the computational cost for the 2-point ERBM is very much cheaper compared to the existing rational methods.

There are a few unusual observations that draw our attentions. From Table 2, the rational method by van Niekerk [21] and 2-point ERBM do not return satisfying results for N = 100, as if these methods cannot approximate *Problem 2* accurately for step-size h = 0.1. As *Problem 2* is a very stiff problem, step-size that is less than 0.1, is required so that a numerical method can approximate accurately the solutions that are varying rapidly with x.

For *Problem 3*, the solutions generated by the rational method of van Niekerk [22] are unstable for N = 160 and N = 320. Smaller step-size is required to satisfy the step-size restriction set by the rational method of van Niekerk [22]. The result generated by the third order rational method of van Niekerk [21] for N = 320, is an unexpected

one, and the cause to this is yet to be identified.

# 6.2 Variable Step-size Approach

Table 6 until Table 10 showed the numerical comparisons of various third order rational methods which obtained using the variable step-size strategy. We also provide the initial step-size ( $h_0$ ) for each problem being solved.

**Table 6:** Comparisons of various third order rational methods in solving *Problem 1*  $(h_0 = 0.1)$ 

TOL	METHOD	SSTEP	<b>FSTEP</b>	MAXE
	van Niekerk [21]	5	0	4.88854(-03)
10-2	van Niekerk [22]	5	0	1.72972(-04)
$10^{-2}$	Ramos [26]	5	0	1.43693(-03)
	2-point ERBM	3	0	7.69877(-05)
	van Niekerk [21]	49	18	1.16717(-04)
10-4	van Niekerk [22]	6	2	1.10009(-04)
$10^{-4}$	Ramos [26]	13	9	1.15537(-04)
	2-point ERBM	3	0	7.69877(-05)
	van Niekerk [21]	332	28	1.14899(-06)
$10^{-6}$	van Niekerk [22]	33	8	1.13273(-06)
	Ramos [26]	64	15	1.14626(-06)
	2-point ERBM	8	4	5.16657(-06)

From Table 6, all existing third order rational methods require 5 successful steps within the interval [0,0.5] when the prescribed tolerance is  $10^{-2}$ . However, 2-point ERBM turned out to have better accuracy and smaller number of successful steps compared to other existing third order rational methods in solving *Problem 1*. When the prescribed tolerance is decreased to  $10^{-4}$ , there is a great increase in the number of successful steps for the third order method of van Niekerk [21] and a slight increase in the number of successful steps for the third order method of Ramos [26]. On the other hand, the number of successful steps for the methods of van Niekerk [22] and 2-point ERBM remain (or almost) unchanged. In the case when the prescribed tolerance is  $10^{-4}$ , 2-point ERBM also turned out to have better accuracy compared to other existing third order rational methods. When the prescribed tolerance is  $10^{-6}$ , all third order methods are found to have comparable accuracy but with different number of successful steps within [0,0.5]. We can see that 2-point ERBM is the cheapest in computational cost, followed by van Niekerk [22], Ramos [26], and lastly van Niekerk [21].

**Table 7:** Comparisons of various third order rational methods in solving *Problem 2*  $(h_0 = 0.0001)$ 

TOL	METHOD	SSTEP	FSTEP	MAXE
	van Niekerk [21]	10001	0	1.89317(-06)
10-2	van Niekerk [22]	10001	0	1.10728(-06)
$10^{-2}$	Ramos [26]	10001	0	1.44295(-05)
	2-point ERBM	5001	0	2.19011(-08)
	van Niekerk [21]	10001	0	1.89317(-06)
10-4	van Niekerk [22]	10001	0	1.10728(-06)
$10^{-4}$	Ramos [26]	10001	0	1.44295(-05)
	2-point ERBM	5001	0	2.19011 (-08)
	van Niekerk [21]	-	-	-
$10^{-6}$	van Niekerk [22]	10001	0	1.10728(-06)
	Ramos [26]	-	-	-
	2-point ERBM	5001	0	2.19011 (-08)

The initial step-size of *Problem 2* is set to  $h_0 = 0.0001$  so that stability and convergence of numerical solution generated by all third order rational methods are guaranteed under specific prescribed tolerance. With this initial step-size, we observed from Table 7 that, all existing third order rational methods required 10001 successful steps within the interval [0,1]; meanwhile the 2-point ERBM only needs 5001 successful steps for all three prescribed tolerances i.e.  $10^{-2}$ ,  $10^{-4}$  and  $10^{-6}$ . Hence, the generated maximum absolute relative errors for every prescribed tolerance are found to be identical. We can see that the 2-point ERBM is the cheapest in computational cost and is able to generate more accurate results compared to other existing third order rational methods. We wish to point out that: third order method of van Niekerk [21] failed to converge, while third order method of Ramos [26] suffered too many step-size rejections when the accepted error estimate is set to be bounded by 10<sup>-6</sup>. Therefore, there are a few things that need to be considered when solving nonautonomous stiff problem using rational methods with variable step-size i.e., careful selection of initial step-size and looser prescribed tolerance if high accuracy is unnecessary.

**Table 8:** Comparisons of various third order rational methods in solving *Problem 3*  $(y_1(x))$   $(h_0 = 0.1)$ 

TOL	METHOD	SSTEP	FSTEP	MAXE
	van Niekerk [21]	324	5	4.73073(-03)
$10^{-2}$	van Niekerk [22]	347	5	3.04129(-03)
10	Ramos [26]	675	5	4.82570(-03)
	2-point ERBM	282	5	8.57747(-03)
	van Niekerk [21]	-	-	-
1.0-4	van Niekerk [22]	-	-	-
$10^{-4}$	Ramos [26]	831	5	4.22516(-05)
	2-point ERBM	-	-	-
	van Niekerk [21]	1079	16	1.13313(-06)
1.0-6	van Niekerk [22]	1108	9	1.14692(-06)
$10^{-6}$	Ramos [26]	842	5	4.46487(-07)
	2-point ERBM	1926	6	4.87328(-06)

**Table 9:** Comparisons of various third order rational methods in solving *Problem 3*  $(y_2(x))$   $(h_0 = 0.1)$ 

TOL	METHOD	SSTEP	FSTEP	MAXE
	van Niekerk [21]	324	5	7.86713(-03)
$10^{-2}$	van Niekerk [22]	347	5	8.74745(-03)
10	Ramos [26]	675	5	4.83053(-03)
	2-point ERBM	282	5	1.32171(-02)
	van Niekerk [21]	-	_	-
1.0-4	van Niekerk [22]	-	-	-
$10^{-4}$	Ramos [26]	831	5	9.12470(-05)
	2-point ERBM	-	-	-
	van Niekerk [21]	1079	16	1.13210(-06)
$10^{-6}$	van Niekerk [22]	1108	9	1.14692(-06)
	Ramos [26]	842	5	9.11908(-07)
	2-point ERBM	1926	6	9.33509(-06)

Problem 3 is a mildly stiff problem. From Table 8 and Table 9, and when the tolerance is  $10^{-2}$ , we have observed that all third order methods are comparable in accuracy in computing the components  $y_1(x)$  and  $y_2(x)$ , except for 2-point ERBM. We can see that 2-point ERBM is the cheapest in computational cost, followed by van Niekerk [21], van Niekerk [22], and lastly Ramos [26]. When the tolerance is decreased to  $10^{-4}$ , we observed that only the third order rational method by Ramos [26] returned the results for both components. The remaining third order rational methods suffer from pro-long integration process due to very excessive small step-

sizes. Finally, when the prescribed tolerance is set to  $10^{-6}$ , we can see that the third order rational method by Ramos [26] is the cheapest in computational cost and is able to generate more accurate results compared to other existing third order rational methods, in computing both component  $y_1(x)$  and  $y_2(x)$ . Surprisingly, the 2-point ERBM requires the most integration step in order to achieve the accuracy comparable to van Niekerk [21] and van Niekerk [22].

**Table 10:** Comparisons of various third order rational methods in solving *Problem 4*  $(h_0 = 0.1)$ 

TOL	METHOD	SSTEP	FSTEP	MAXE
	van Niekerk [21]	1611	5	7.79836(-05)
1.0-2	van Niekerk [22]	958	4	7.88256(-05)
$10^{-2}$	Ramos [26]	521	3	3.66823(-04)
	2-point ERBM	555	4	7.41100(-05)
	van Niekerk [21]	10667	8	1.06762(-07)
10-4	van Niekerk [22]	4334	7	1.03121(-06)
$10^{-4}$	Ramos [26]	1893	5	7.35386(-06)
	2-point ERBM	1601	5	1.01853(-06)
	van Niekerk [21]	80389	14	5.74256(-09)
6	van Niekerk [22]	21856	12	1.07760(-08)
$10^{-6}$	Ramos [26]	9781	10	1.13378(-07)
	2-point ERBM	4817	8	2.20735(-08)

Problem 4 is a mildly stiff system arises from the reduction of a second order initial value problem to a system of coupled first order differential equations. From Table 10, when the prescribed tolerance is  $10^{-2}$ , we can see that the computational cost of the 2-point ERBM and the third order rational method of Ramos [26] is relatively lower compare to the computational cost of the third order rational methods of van Niekerk [21] and van Niekerk [22]. The 2-point ERBM generated result with an accuracy of 10<sup>-4</sup> with much more lower computational cost. When the tolerance is decreased to 10<sup>-4</sup>, the 2-point ERBM or the third order rational method by Ramos [26] is cheaper in computational cost if an accuracy of 10<sup>-6</sup> is desired. Alternatively, one can choose the third order method of van Niekerk [21] if an accuracy of  $10^{-7}$  is preferable with 10667 successful steps. However, we would not recommend the third order method of van Niekerk [21] due to its large number of successful steps, unless higher accuracy is desired. Finally, when the prescribed tolerance is further decreased to  $10^{-6}$ , it seems to have a few options based on our point of view. For example, if computational cost is our main concern, then the 2-point ERBM could be a good choice. If our only concern is the accuracy, then the third order rational method by van Niekerk [21] could be our choice.

# **CONCLUSIONS**

The aims of this paper are two folds: i) to introduce the idea of block methods that are based on rational functions, and ii) to provide the rationale that motivates the concepts and developments of rational block methods (RBMs). In order to illustrate the concept of RBM, a 2-point explicit rational block method (2-point ERBM) is introduced in this paper. The 2-point ERBM is able to approximate two successive solutions at the points  $x_{n+1}$  and  $x_{n+2}$  defined in the same block (see Figure 1), within every single integration step. The 2-point ERBM also contained two rational formulae, and both formulae are found to possess third order of accuracy. Figure 2 showed that the 2-point ERBM has a finite region of absolute stability and concluded that it is not A-stable. Numerical experiments showed that the 2-point ERBM generated converging numerical solutions. In most of the test problems, the 2-point ERBM generated numerical solutions with better accuracy and cheaper computational cost in both constant step-size and variable step-size approaches.

Finally, this is the pilot study of RBM, and many more RBMs will be developed in the near future. From the rational approximant in (5), we can see that the degree of the numerator is greater than the degree of the denominator. We believed that this kind of selection yields method with finite region of absolute stability. In order to develop A-stable RBM, we should consider a rational approximant with both numerator and denominator in equal degree. Of course, L-stable RBM may be developed if the underlying rational approximant has the degree of denominator greater than the degree of numerator. All of these directions constitute a vast research dimensions to be explored in the near future.

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