NEW RATIONAL METHODS FOR THE NUMERICAL SOLUTION OF FIRST ORDER INITIAL VALUE PROBLEM

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PENGAKUAN TANGGUNGJAWAB (DICLAIMER)

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ABSTRACT

Exponentially-fitted numerical methods are appealing because L-stability is guaranteed when solving initial value problems of the form $y' = \lambda y$, $y(a) = \eta$, $\lambda \in \mathbb{C}$, $\mathrm{Re}(\lambda) < 0$. Such numerical methods also yield the exact solution when solving the above-mentioned problem. Whilst rational methods have been well established in the past decades, most of them are not 'completely' exponentially-fitted. Recently, a class of one-step exponential-rational methods (ERMs) were discovered. Analyses showed that all ERMs are exponentially-fitted, hence implying L-stability. Several numerical experiments showed that ERMs is more accurate than existing rational methods in solving general initial value problem. However, ERMs have several weaknesses: i) every ERM is non-uniquely defined; ii) may return complex values; and iii) less accurate numerical solution when solving problem whose solution possesses singularity. Therefore, the first purpose of this study is to modify the original ERMs so that the first two weaknesses will be overcomed. Theoretical analyses such as consistency, stability and convergence of the modified ERMs are presented. Numerical experiments showed that the modified ERMs and the original ERMs are found to have comparable accuracy; hence modified ERMs are preferable to original ERMs. The second purpose of this study is to overcome the third weakness of the original ERMs where a variable step-size strategy is proposed to improve the accuracy ERMs. The procedures of the strategy are detailed out in this report. Numerical experiments have revealed that the affects from the implementation of the strategy is less obvious.

Keywords: Exponential-rational method, Modified exponential-rational method, Variable-step-size strategy.

ABSTRAK

Kaedah-kaedah berangka yang bersesuaian secara eksponen adalah menarik kerana kestabilan *L* adalah terjamin apabila menyelesaikan masalah nilai awal yang berbentuk $y' = \lambda y$, $y(a) = \eta$, $\lambda \in \mathbb{C}$, $\mathrm{Re}(\lambda) < 0$. Kaedah-kaedah berangka yang sedemikian juga menghasilkan penyelesaian tepat apabila menyelesaikan masalah yang dinyatakan di atas. Walaupun kaedah-kaedah nisbah telah menjadi mantap dalam beberapa dekad yang lalu, sebahagian besar daripada kaedah-kaedah ini tidak bersesuian secara eksponen sepenuhnya. Baru-baru ini, satu kelas kaedah-kaedah eksponen-nisbah satu-langkah (ERM) telah ditemui. Beberapa analisis menunjukkan bahawa semua ERM adalah bersesuaian secara eksponen, maka mengimplikasikan kestabilan *L*. Beberapa pengujian berangka menunjukkan bahawa ERM adalah lebih tepat berbanding dengan kaedah-kaedah nisbah yang sedia ada dalam menyelesaikan masalah nilai awal umum. Walau bagaimanapun, ERM mempunyai beberapa kelemahan: i) setiap ERM tidak ditakrifkan secara unik; ii) boleh mengembalikan nilai-nilai yang kompleks; dan iii) penyelesaian berangka yang kurang tepat apabila menyelesaikan masalah yang penyelesaiannya mempunyai ketunggalan. Oleh itu, tujuan pertama kajian ini adalah untuk mengubah suai ERM yang asal supaya dua kelemahan yang pertama akan diatasi. Analisis teori seperti kekonsistenan, kestabilan dan penumpuan bagi ERM yang diubahsuai dibentangkan. Pengujian secara berangka menujukkan bahawa ERM yang telah diubahsuai dan ERM yang asal didapati mempunyai ketepatan yang setara; maka ERM yang diubahsuai lebih sesuai berbanding ERM yang asal. Tujuan kedua kajian ini adalah untuk mengatasi kelemahan ketiga ERM yang asal, di mana satu strategi saiz-langkah boleh ubah telah diperkenalkan untuk meningkatkan ketepatan ERM. Prosedur strategi telah dinyatakan secara terperinci dalam laporan ini. Pengujian secara berangka telah menunjukkan bahawa kesan daripada pelaksanaan strategi ini adalah kurang jelas.

Kata-kata kunci: Kaedah eksponen-nisbah, Kaedah eksponen-nisbah diubahsuai, Strategi saiz-langkah boleh ubah.

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CHAPTER ONE

INTRODUCTION

1.1 Background of the Study

We consider the numerical solution of the initial value problem

$$y'(x) = f(x, y), \quad y(a) = \eta. \tag{1.1}$$

If the solution of (1.1) is known to be periodic or oscillate with a known frequency, then a numerical integration formulae based on trigonometric functions is appropriate (Lambert, 1973). On the other hand, if the solution of (1.1) possesses singularities, then a numerical integration formulae based on rational functions will be much more effective. In both cases, unconventional methods are preferable as they adapt to the structure or to the solution of the problem better than conventional methods.

Unconventional methods are special numerical methods which are developed to solve certain types of initial value problems, where in the main, conventional methods such as linear multistep methods and Runge-Kutta methods will perform poorly. Besides incorporating trigonometric functions and rational functions as non-polynomial interpolants to form new special methods, other commonly used non-polynomial interpolants are logarithmic functions and exponential functions. For excellent surveys and various perspectives on numerical methods based on various non-polynomial interpolants, refer to Lambert & Shaw (1965), Shaw (1967), Lambert (1973), Lambert (1974), Luke *et al*. (1975), Fatunla (1976), Wambecq (1976), Evans & Fatunla (1977), Fatunla (1978), Lee & Preiser (1978), Fatunla (1982), Fatunla (1986), Van Niekerk (1987), Van Niekerk (1988), Wu (1998), Wu &

Xia (2000a), Wu & Xia (2000b), Wu & Xia (2001), Ikhile (2001), Ikhile (2002), Wu & Xia (2003), Ikhile (2004), Ramos (2007), Okosun & Ademiluyi (2007a), Okosun & Ademiluyi (2007b), Teh *et al*. (2009), Yaacob *et al.* (2010), Teh (2010), Teh *et al.* (2011), Teh & Yaacob (2013a), and Teh & Yaacob (2013b).

1.2 Statement and Scope of the Study

All the works mentioned above have discussed various formulations of one-step rational methods as well as some rational methods in a multistep setting that are based on various forms of rational interpolants. These rational interpolants possess either both numerator and denominator being polynomial expressions or only one of them is a polynomial expression. However, Teh (2010) and Teh & Yaacob (2013b) suggested that the incorporation of exponential function into conventional rational function to form a new kind of rational interpolant in developing a rational method with special properties. The resulting methods are rational methods that are exponentially-fitted because they yield exact solutions when solving the problem

$$y' = \lambda y,\ y(a) = \eta,\ \lambda \in \mathbb{C},\ \mathrm{Re}(\lambda) < 0. \tag{1.2}$$

These exponentially-fitted methods are known as one-step exponential-rational methods (ERMs) which suggest an approximation to the theoretical solution of (1.1) at x_{n+1} is given by

$$y_{n+1} = \frac{\sum_{i=0}^{k} a_i h^i + c_1 e^{c_2 h}}{1 + bh},\ 1 + bh \neq 0. \tag{1.3}$$

where b, c_1, c_2 and a_j for $j = 0,1,\ldots,k$ are parameters that may contain $y(x_n)$ and higher derivatives of $y(x_n)$. Note that $a_j = 0$ if k is set to 0. If an ERM has order *p*, then this particular ERM is called a *p*-ERM. Teh (2010) developed all ERMs of order

2 until order 5, together with their respective local truncation errors and stability functions. Stability analyses had showed that all ERMs developed are *L*-stable. Furthermore, all ERMs proposed were compared numerically with those existing rational methods in the articles mentioned above, using some test problems. Numerical results showed that almost all ERMs gave more accurate numerical solutions in solving (1.1).

However, some of the ERMs are less accurate if compared to the existing rational methods of Ikhile (2001) and Ramos (2007) when solving problem in (1.1) whose solution possesses singularity. A solution to this could be found in the works by Ikhile (2002) and Ikhile (2004). Ikhile (2002) considered an extrapolation method involving rational method as basic integrator and a variable step-size strategy was embedded. A similar approach was considered in Ikhile (2004). Findings from both papers showed that extrapolation approaches with step-size control are more accurate than those extrapolation approaches with constant step-size especially in solving problem whose solution possesses singularity. In view of this, with the variation in the step-size, the numerical results of ERMs can be improved when solving problem (1.1) whose solution possesses singularity. Therefore, a variable step-size strategy will be introduced in this study for numerical implementations purposes.

Despite the strong stability characteristics and better accuracies of ERMs in (1.3), there are two shortcomings of ERMs. Firstly, there are actually two different ERMs for each order of accuracy due to the fact that two different expressions of c_2 emerged during the derivation process. In other words, a *p*-th order ERM is not unique but two different methods. At this moment, no criterion or condition has been devised to determine which ERM is better for the same order of accuracy. In view of this, we wish to modify the original ERM of Teh (2010) and Teh & Yaacob (2013b) so that the modified ERM will yield only one method for each order of accuracy.

Secondly, the parameter c_2 of each ERM in (1.3) may contain an expression with square root. In other words, there are times where ERM will produce numerical solutions that are complex numbers due to the square root evaluations of the parameter c_2. In order to retrieve numerical solutions that are only real numbers, Teh (2010) and Teh & Yaacob (2013b) chose to consider the real parts of the resulting complex values and ignored the imaginary parts of the complex values that were found numerically to be very small. However, by ignoring the imaginary parts of the complex values will somehow affect the degree of accuracy of the numerical solutions. Therefore, we wish to modify the original ERM of Teh (2010) and Teh & Yaacob (2013b) so that the modified ERM does not involve square root evaluations but at the same time retain the *L*-stability.

1.3 Objectives of the Study

From the statements and scopes made in Section 1.2, it is clear that our main objectives are:

a) To develop a new class of one-step modified exponential-rational methods for the numerical solutions of (1.1); and
b) To develop a strategy of variation in step-size for the new modified exponential-rational methods as well as for those existing one-step rational methods.

1.4 Significance of the Study

This research is of significance to the domain of unconventional methods based on rational functions as it extends the knowledge that currently exists in that field. This is because a new class of one-step modified exponential-rational methods that are free from the shortcomings of the original exponential-rational methods, is derived. At present, these kind of rational methods have never been reported elsewhere. Another important discovery is that the variation step-size strategy for conventional one-step method such as Runge-Kutta method, can be easily extended to unconventional one-step method such as one-step rational method.

1.5 Outline of Report

In Chapter 2, we review some rational methods found in the literature, together with their rational interpolants, local truncation error analyses and stability analyses.

Chapter 3 is about the developments of a new class of modified exponential-rational methods. Generalizations of the new methods, corresponding local truncation errors and absolute stability analyses are presented. Generalized order of consistency and convergence are also presented. An example of modified exponential-rational method is generated and compared with other existing rational methods in the same order in solving some test problems.

Chapter 4 is about the implementation of variation step-size strategy on rational methods. Numerical experimentations are carried out to illustrate the efficiency of the variation step-size strategy in improving the numerical accuracy.

Chapter 5 contains some summaries of our findings in this study and several recommendations for future research.

CHAPTER TWO

LITERATURE REVIEWS

2.1 Introduction

In this chapter, an introduction to the first order initial value problems will be carried out in the next section, followed by an extensive discussion on unconventional methods that are based on rational functions. We also note that the variables '*h*' appear in this chapter and the following chapters are referred as step-size of numerical methods.

2.2 Initial Value Problems For First Order Ordinary Differential Equations

A first order ordinary differential equation $y'(x) = f(x, y)$ together with an initial condition constitutes an initial value problem

$$y'(x) = f(x, y), \quad y(a) = \eta. \tag{2.1}$$

The most important theorem is the standard theorem which states the sufficient conditions for a unique solution of (2.1) to exist. This theorem is given as below (Lambert, 1991):

Theorem 2.1 (*Existence of unique solution of an initial value problem*)

Let $f(x, y)$, *where* $f : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, *be defined and continuous for all* (x, y) *in the region D defined by* $a \le x \le b$, $-\infty < y < \infty$, *a and b are finite, and let there exists a constant L such that*

$$\left| f(x, y) - f(x, y^*) \right| \le L \left| y - y^* \right| \tag{2.2}$$

holds for every $(x,y),(x,y^*)\in D$. *Then for any* $\eta\in\mathbb{R}$, *there exists a unique solution* $y(x)$ *of the problem (2.1) where* $y(x)$ *is continuous and differentiable for all* $(x,y)\in D$.

The requirement (2.2) is known as a Lipschitz condition and the constant L as a Lipschitz constant. If $f(x,y)$ is differentiable with respect to *y*, then from the mean value theorem

$$f(x,y)-f(x,y^*)=\frac{\partial f(x,\bar{y})}{\partial y}(y-y^*), \tag{2.3}$$

where $\bar{y}$ is a point in the interior of the interval whose end-points are *y* and y^*, and (x,y), (x,y^*) are both in the region *D* (Lambert, 1973). Therefore, if we choose

$$L=\sup_{(x,y)\in D}\left|\frac{\partial f(x,y)}{\partial y}\right|, \tag{2.4}$$

then condition (2.2) of Theorem 2.1 is satisfied (Lambert, 1973).

If there are more than one first order ordinary differential equations that need to be solved at one time, then we are facing a system of *m* simultaneous first order ordinary differential equations in *m* dependent variables y_1, y_2, …, y_m. If each of these variables is defined at the same initial point, then we have an initial value problem for a first order system (Lambert, 1991)

$$\begin{aligned}
y_1' &= f_1(x,y_1,y_2,\ldots,y_m),\ y_1(a)=\eta_1,\\
y_2' &= f_2(x,y_1,y_2,\ldots,y_m),\ y_2(a)=\eta_2,\\
&\ \ \vdots \qquad\qquad\qquad\qquad \vdots\\
y_m' &= f_m(x,y_1,y_2,\ldots,y_m),\ y_m(a)=\eta_m.
\end{aligned} \tag{2.5}$$

For simplicity, system (2.5) can also be expressed in vector form by introducing the following vector notation:

$$\mathbf{y} = \begin{pmatrix} y_1 & y_2 & \cdots & y_m \end{pmatrix}^{\mathrm{T}},$$

$$\mathbf{y}' = \begin{pmatrix} y_1' & y_2' & \cdots & y_m' \end{pmatrix}^{\mathrm{T}},$$

$$\mathbf{f}(x,\mathbf{y}) = \begin{pmatrix} f_1(x, y_1, y_2, \ldots, y_m) \\ f_2(x, y_1, y_2, \ldots, y_m) \\ \vdots \\ f_m(x, y_1, y_2, \ldots, y_m) \end{pmatrix},$$

$$\mathbf{y}(a) = \begin{pmatrix} y_1(a) \\ y_2(a) \\ \vdots \\ y_m(a) \end{pmatrix},$$

and

$$\boldsymbol{\eta} = \begin{pmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ \eta_m \end{pmatrix}.$$

Hence, the vector form of system (2.5) is

$$\mathbf{y}' = \mathbf{f}(x,\mathbf{y}), \quad \mathbf{y}(a) = \boldsymbol{\eta}. \tag{2.6}$$

Theorem 2.1 readily generalizes to give necessary conditions for the existence of a unique solution to system (2.6); where the region D is now defined by $a \le x \le b$, $-\infty < y_i < \infty$ for $i = 1, 2, \ldots, m$, and conditions (2.2) is replaced by the condition

$$\left\| \mathbf{f}(x,\mathbf{y}) - \mathbf{f}(x,\mathbf{y}^*) \right\| \le L \left\| \mathbf{y} - \mathbf{y}^* \right\|, \tag{2.7}$$

where $(x,\mathbf{y})$ and $(x,\mathbf{y}^*)$ are in D, and $\| \cdot \|$ denotes a vector norm (Lambert, 1973). If $\mathbf{f}(x,\mathbf{y})$ is differentiable with respect to **y**, then from the mean value theorem

$$\mathbf{f}(x,\mathbf{y})-\mathbf{f}(x,\mathbf{y}^*)=\frac{\partial\mathbf{f}(x,\bar{\mathbf{y}})}{\partial\mathbf{y}}(\mathbf{y}-\mathbf{y}^*), \tag{2.8}$$

where the notation implies that each row of the Jacobian $\partial\mathbf{f}(x,\bar{\mathbf{y}})/\partial\mathbf{y}$ is evaluated at different mean values which are internal points of the line segment from $(x,\mathbf{y})$ to $(x,\mathbf{y}^*)$, all of which are points in region D (Lambert, 1973). Therefore, if we choose

$$L=\sup_{(x,\mathbf{y})\in D}\left\|\frac{\partial\mathbf{f}(x,\mathbf{y})}{\partial\mathbf{y}}\right\|, \tag{2.9}$$

then condition (2.7) is satisfied (Lambert, 1991).

Some of the solutions of scalar problem (2.1) and system (2.6) can be obtained analytically. When an initial value problem can be solved analytically, then this particular problem has one theoretical solution for (2.1) and m theoretical solutions for (2.6). Numerical integration formulae for problems (2.1) and (2.6) are used when they cannot be solved analytically, where theoretical solution(s) cannot be obtained. Numerical integration formulae will give approximate solutions for the theoretical solutions. There are three popular integration methods for problems (2.1) and (2.6). We can either use linear multistep methods, predictor-corrector methods or Runge-Kutta methods to obtain the approximations for initial value problems. These numerical methods are classical numerical methods and can be found in most text books on numerical solutions of initial value problems. For more information on conventional numerical methods for initial value problems, see Henrici (1962), Milne (1970), Gear (1971), Stetter (1973), Lambert (1973), Jain (1984), Butcher (1987), Fatunla (1988), Lambert (1991), Hairer & Wanner (1991), Hairer *et al*. (1993), Iserles (1996) and Butcher (2003).

2.3 Unconventional Methods Based On Rational Functions

Let us consider the initial value problems (2.1) where y, $f \in \mathbb{R}$ and $x \in [a,b]$ a finite interval on the real line. Conventional one-step scheme is given by

$$y_{n+1} = y_n + h\phi(x_n, y_n, h) \tag{2.10}$$

where $\phi(x_n, y_n, h)$ is the increment function; and conventional linear multistep method is described by

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\sum_{j=0}^{k} \beta_j f_{n+j} \tag{2.11}$$

where α_j and β_j are real coefficients. The basic formulation of (2.10) and (2.11) is based on the local representation of a polynomial of the theoretical solution to (2.1). If (2.10) and (2.11) were used to pursue the numerical solutions that possess singularities, then (2.10) and (2.11) fail woefully near the singular points (Lambert, 1973; Fatunla, 1982; Van Niekerk, 1988; and Ikhile, 2001). This is because (2.10) and (2.11) are formulated on the basis that the initial value problems (2.1) satisfy the existence and uniqueness theorem, so that polynomial interpolation can be applied quite successfully in the formulation (Ikhile, 2001).

A natural step would appear to be the replacement of the polynomial function for both (2.10) and (2.11), by a rational function due to its smooth behaviour in the neighbourhood of singularities (Ikhile, 2001). Lambert & Shaw (1965) were the first researchers to use rational interpolant in developing one-step rational methods that are suitable to solve (2.1) whose solutions possess singularities. Lambert & Shaw (1965) had assumed that the theoretical solution of (2.1) can be represented locally in the interval $[x_n, x_{n+1}]$ by the rational interpolant of the form (Wambecq, 1976)

$$F(x)=\frac{P_n(x)}{b+x} \tag{2.12}$$

where $P_n(x)=\sum_{i=0}^{n}a_i x^i$ is a polynomial of degree *n*; *b* and a_i for $i=0,1,\ldots,n$ are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$. On imposing the requirements that $y_n=F(x_n)$, $y_{n+1}=F(x_{n+1})$ and $f_n^{(s)}=F^{(s)}(x_n)$, one gets a class of one-step explicit rational methods based on interpolant (2.12) which involve the first $(s+1)$ derivatives of *y*, which is given by (Lambert, 1973)

$$y_{n+1}=y_n+\sum_{i=1}^{s}\frac{h^i}{i!}y_n^{(i)}+\frac{h^{s+1}}{s!}\frac{y_n^{(s)}y_n^{(s+1)}}{(s+1)y_n^{(s)}-hy_n^{(s+1)}},\ s=0,1,2,\ldots, \tag{2.13}$$

where, in the case $s=0$, the term $\sum_{i=1}^{s}\frac{h^i}{i!}$ is taken to be zero. The local truncation error of (2.13) is

$$\frac{h^{s+2}}{(s+2)!}\left[y^{(s+2)}(x_n)-\frac{s+2}{s+1}\frac{\left(y^{(s+1)}(x_n)\right)^2}{y^{(s)}(x_n)}\right]+O\left(h^{s+3}\right), \tag{2.14}$$

and we can say that method (2.13) has order $s+1$. Each method of the class (2.13) is seen to be truncated Taylor series with a rational correcting term (Lambert, 1973). On applying (2.13) to the test equation given in (1.2), the stability functions of method (2.13) for $s=0,1,2,\ldots$ can be easily obtained. The value *s* decides the number of derivatives to be evaluated in (2.13) i.e. a total of $y_n^{(m)}$ for $m=1,2,\ldots,s,s+1$. The higher the value of *s*, the more derivatives evaluations need to be carried out, which might be time consuming especially in solving large scale problems. Lambert & Shaw (1965) also showed that implicit one step formulae, explicit and implicit multistep formulae were possible based on interpolant (2.12).

According to Fatunla (1986), Fatunla (1988), Ikhile (2001) and Ikhile (2004), the very first multistep method based on rational interpolant was developed by Luke *et al*. (1975). Luke *et al*. (1975) suggested a replacement of the rational interpolant (2.12) by the generalized rational function

$$F(x) = \frac{P_m(x)}{Q_n(x)} \tag{2.15}$$

where $P_m(x) = \sum_{i=0}^{m} a_i x^i$ and $Q_n(x) = 1 + \sum_{i=1}^{n} b_i x^i$ are polynomials of degree *m* and *n* respectively. We note that a_i and b_i , are parameters that may contain approximations of $y(x_{n+j})$ and higher derivatives of $y(x_{n+j})$ for $j = 0(1)k$, where *k* is the step number. Luke *et al*. (1975) had developed the simplest two-step predictor-corrector formulae given by

$$y_{n+2} = \frac{2y_n y_{n+1} - 2(y_{n+1})^2 + hy_n y'_{n+1}}{2y_n - 2y_{n+1} + hy_{n+1}} \tag{2.16}$$

and

$$y_{n+2} = \frac{(y_{n+1})^2 - h^2 y'_{n+1} y'_{n+2}}{2y_{n+1} - y_{n+2}} \tag{2.17}$$

respectively. According to Fatunla (1986) and Ikhile (2004), higher order formulae are quite unwieldy and their generalized formulations are almost impossible. The approach to derive these predictor-corrector methods can be found in Luke *et al*. (1975), Fatunla (1986), Fatunla (1988) and Ikhile (2004).

Later, Lambert (1974) also quoted a selection of one-step rational methods based on some specifications of rational interpolant given by (2.15). In the case of one-step methods, we note that a_i and b_i of (2.15) are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$. On the other hand, in the case of multistep methods, we note that a_i and b_i are parameters that may contain approximations of $y\left(x_{n+j}\right)$ and higher derivatives of $y\left(x_{n+j}\right)$ for $j=0(1)(k-1)$, where k is the step number. Lambert (1974) had quoted five examples of one-step rational methods and two examples of 2-step rational methods, together with their corresponding order conditions and stability properties. All of these methods in Lambert (1974) are all component applicable to the system (2.6). For those who are interested with these methods, one can refer to Lambert (1974).

For the discussion of order condition, we pick the simplest form derived from rational function $F(x)=a_0/(b_0+x)$ i.e.

$$y_{n+1}=y_n+\frac{hy_n y'_n}{y_n-hy'_n}. \tag{2.18}$$

Method (2.18) can also be obtained by using $s=0$ in equation (2.13). From (2.18), there are two things that we need to take good care of. Firstly, $y(x)$ and $y'(x)$ of initial value problems (2.1) must not vanish simultaneously (Lambert, 1974). Secondly, if h is such that $y_n-hy'_n$ vanishes, we must choose another value for h (Lambert, 1974). Similar to the usual procedure for linear multistep methods, we can associate a non-linear operator with each rational method derived from (2.15). For method (2.18), the operator is $P\left[z(x);h\right]$ defined as

$$P\left[z(x);h\right]=z(x+h)-z(x)-\frac{hz(x)z'(x)}{z(x)-hz'(x)},$$

where $z(x)$ is an arbitrary function such that $z(x)$ and $z'(x)$ do not vanish simultaneously for all $x\in[a,b]$ (Lambert, 1974). If $P\left[z(x);h\right]=O\left(h^{p+1}\right)$ for sufficiently differentiable $z(x)$, we can say that the method has order p, and the local truncation error is $T_{n+1} = P\left[y(x_n); h \right]$, where $y(x)$ is now taken to be the theoretical solution of the initial value problems. Lambert (1974) had proven that method (2.18) is *L*-stable. Below is the definition of *A*-stability follow by the definition of *L*-stability (Lambert, 1973):

Definition 2.1 (*A-stability*)

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

Definition 2.2 (*L-stability*)

A one-step numerical method is said to be L-stable if it is A-stable and, in addition, when applied to the scalar test equation $y' = \lambda y$, λ *a complex constant with* $\operatorname{Re} \lambda < 0$, *it yields* $y_{n+1} = R(h\lambda) y_n$, *where* $|R(h\lambda)| \to 0$ *as* $\operatorname{Re} h\lambda \to -\infty$. h *is the step length and* $R(h\lambda)$ *is the stability function for the one-step method.*

Besides multistep methods mentioned in Lambert (1974) and those from Luke *et al*. (1975), Fatunla (1982) had suggested that the theoretical solution of (2.1) is locally approximated by

$$F_k(x) = \frac{A}{1 + \sum_{r=1}^{k} a_r x^r}, \tag{2.19}$$

where A and a_r for $r = 1(1)k$ are parameters that may contain approximations of $y(x_{n+j})$ and higher derivatives of $y(x_{n+j})$ for $j = 0(1)(k-1)$, where k is the step number. The resultant algorithms are *k*-step explicit rational methods for general initial value problems as well as problems whose solutions possess singularities. The singularities are the poles of (2.19) and could be overstepped by adjusting the step-size (Fatunla, 1982). The proposed algorithms are stable and their order corresponds with the step number *k* (Fatunla, 1982).

Consider the case when the denominator of (2.19) is linear, that is $k=1$. Since the order corresponds with the step number *k*, therefore the explicit one-step method derived from (2.19) will always have order 1. This one-step explicit method is given by

$$y_{n+1}=\frac{\left(y_n\right)^2}{\left(y_n-hy'_n\right)}. \tag{2.20}$$

The non-linear operator $P\left[z(x);h\right]$ associate with method (2.20) is specified by

$$P\left[z(x);h\right]=z(x+h)-\frac{z(x)^2}{z(x)-hz'(x)}, \tag{2.21}$$

where $z(x)$ is an arbitrary function with the constraint that $z(x)$ and $z'(x)$ do not vanish simultaneously for all $x\in[a,b]$. The method (2.20) is said to be of order *p* if $P\left[z(x);h\right]=O\left(h^{p+1}\right)$ and the local truncation error T_{n+1} is given by $P\left[y(x_n);h\right]$ where $y(x)$ is taken to be the theoretical solution to (2.1). Fatunla (1982) also proposed a 2-step scheme with $k=2$ which yield the following integration formula,

$$y_{n+2}=\frac{\left(1+a_1+a_2\right)^2 y_{n+1}^2}{\left(1+2a_1+4a_2\right)y_n} \tag{2.22}$$

with

$$a_1=-\frac{hy'_n}{y_n} \text{ and } a_2=\frac{\frac{hy'_n}{y_n}\left(hy'_{n+1}+y_{n+1}\right)-hy'_{n+1}}{hy'_{n+1}+2y_{n+1}}.$$

Fatunla (1982) also gave the following generalization of the *k*-step rational methods based on interpolant (2.19) as

$$y_{n+k} = \frac{y_n}{1+\sum_{r=1}^{k} a_r x^r} \tag{2.23}$$

with a_r for $r = 1(1)k$ are parameters that may contain approximations of $y\left(x_{n+j}\right)$ and higher derivatives of $y\left(x_{n+j}\right)$ for $j = 0(1)(k-1)$, where k is the step number. Similar to a linear multistep method, a *k*-step method based on (2.23) also requires $(k-1)$ starting values, which can be generated by one-step method. In Fatunla (1986), method (2.20) was used as the basic integrator to form a polynomial extrapolation scheme and a rational extrapolation scheme. According to Fatunla (1986), the rational extrapolation scheme is more efficient and more accurate than the polynomial extrapolation scheme in solving a problem whose solution possesses singularity.

Van Niekerk (1987) and Van Niekerk (1988) had claimed that the resultant algorithms approximated by the interpolant function (2.19) can only be applied if the initial value $y_0 \neq 0$. While in the case of an initial value $y_0 = 0$, the numerical result will fail at the beginning of the integration. Hence, Van Niekerk (1987) had developed a one-step rational method which can be applied to an initial value problem without any restriction on the initial value. Let the theoretical solution $y(x)$ of (2.1) be approximated by (Van Niekerk, 1987)

$$y_n = a_n + \frac{b_n}{1+c_n x_n} \tag{2.24}$$

where a_n, b_n and c_n are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$. After some algebraic manipulation involving Taylor series expansion of $y(x_{n+1})$, Van Niekerk (1987) developed the following one-step rational method

$$y_{n+1} = y_n + \frac{2h(y_n')^2}{2y_n' - hy_n''}. \tag{2.25}$$

Van Niekerk (1987) had claimed that method (2.25) is a first order method. However, upon careful reviews and inspections, we have found out that method (2.25) is actually a second order method. Hence, we make a correction to the work of Van Niekerk (1987). Method (2.25) has been applied successfully to a problem whose solution possesses singularity and a problem with oscillatory property. Numerical results had shown that method (2.25) produces better results compare to the method (2.22) that proposed by Fatunla (1982), when solving problem whose solution possesses singularity. Algorithm (2.24) can be easily generalized to a higher order algorithm. For instance

$$y_n = \frac{a_n + b_n x_n}{1 + c_n x_n + d_n {x_n}^2}, \tag{2.26}$$

where a_n, b_n, c_n and d_n are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$. According to Van Niekerk (1987), the rational method that developed through the approximation algorithm (2.26) yields a second order method. However, our reviews and inspections reveal that the rational method that developed through the approximation algorithm (2.26) is actually a third order method. Hence, we make another correction to the work of Van Niekerk (1987). Numerical results generated from the method corresponding to (2.26) compare favourably to the numerical results obtained with a fourth order multistep method of Fatunla (1982).

In Van Niekerk (1988), he made another attempt to propose a generalized higher order one-step rational method which can be applied to an initial value problem without any restriction on the initial value. Let the theoretical solution $y(x)$ of (2.1) be approximated by a finite continued fraction defined by

$$T_k(x) = a_0 + \cfrac{a_1 x}{1 + \cfrac{a_2 x}{1 + \cfrac{a_3 x}{1 + \cdots \atop \ddots \; \cfrac{a_k x}{1 + a_{k+1} x}}}}, \tag{2.27}$$

where k denotes the order of the function $T_k(x)$ and a_i for $i = 0, 1, \ldots, k, k+1$ are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$. Van Niekerk (1988) had considered the approximation of $y(x)$ by

$$T_1(x) = y_n = a_0 + \frac{a_1 x_n}{1 + a_2 x_n}, \tag{2.28}$$

where y_n denotes the approximate value of $y(x_n)$, the final integration formula is

$$y_{n+1} = y_n + \frac{2h(y_n')^2}{2y_n' - hy_n''}. \tag{2.29}$$

Notice that (2.29) is identical to (2.25) of Van Niekerk (1987). According to Van Niekerk (1988), the order condition of the method will correspond to the degree of the function (2.27). In other words, method (2.29) should be a first order method because the corresponding function $T_1(x)$ is in first degree. Van Niekerk (1988) also gave the derivations of a second order method which correspond to $T_2(x)$ and a third order method which correspond to $T_3(x)$. However, our reviews and inspections reveal that method (2.29) which based on $T_1(x)$ is not a first order method but actually a second order method; the method correspond to $T_2(x)$ is not a second order method but actually a third order method; and the method correspond to $T_3(x)$ is not a third order method but actually a fourth order method. In view of this, we can say that a method which corresponds to function $T_k(x)$ is a $(k+1)$-th order method. Hence, we make some corrections to the work of Van Niekerk (1988). Van Niekerk (1988) had shown that the structure of a method became more complicated when we increase the order of the method, which also imply increasing the degree of function (2.27). This makes the derivations of higher order methods become more difficult. However, numerical results had shown that these three methods of order 2, 3 and 4, are able to solve problem whose solution possesses singularity, stiff initial value problem and stiff system of non-linear equations accurately.

Ikhile (2001) had considered for the solution of initial value problem (2.1), the rational interpolant is given by

$$y(x) \approx A + \frac{xP_{K-l}(x)}{1+\sum_{j=1}^{K} b_j x^j}, \; K \geq 1, \; l \geq 0, \; K-l \geq 0, \tag{2.30}$$

where

$$P_{K-l}(x) = \sum_{j=0}^{K-l} a_j x^j, \; K \geq 1, \; l \geq 0, \; K-l \geq 0. \tag{2.31}$$

Based on the interpolant in (2.30), Ikhile (2001) had considered the one-step rational method as

$$y_{n+1} = A + \frac{x_{n+1} P_{K-l}\left(x_{n+1}\right)}{1 + \sum_{j=1}^{K} b_j x_{n+1}^j}, \ K \geq 1, \ l \geq 0, \ K - l \geq 0, \tag{2.32}$$

where

$$P_{K-l}\left(x_{n+1}\right) = \sum_{j=0}^{K-l} a_j x_{n+1}^j, \ K \geq 1, \ l \geq 0, \ K - l \geq 0, \tag{2.33}$$

for the initial value problems (2.1) where y_{n+1} and $y\left(x_{n+1}\right)$ are the numerical and theoretical solutions of (2.1) respectively. From (2.32) and (2.33), we note that *A*, b_j for $j = 1(1)K$ and a_j for $j = 0(1)\left(K - l\right)$ are parameters that may contain approximations of $y\left(x_n\right)$ and higher derivatives of $y\left(x_n\right)$. Ikhile (2001) had showed that the attainable order of the method (2.32) is at least $2K - l + 1$. The rational interpolant (2.30) is then specialized to take the form of

$$y\left(x\right) \approx B + \frac{Ax}{1 + \sum_{j=1}^{K} b_j x^j}. \tag{2.34}$$

In the sense of (2.34), Ikhile (2001) had proposed the specialized one-step rational method given by

$$y_{n+1} = B + \frac{Ax_{n+1}}{1 + \sum_{j=1}^{K} b_j x_{n+1}^j}, \tag{2.35}$$

with order of accuracy equals to $K + 1$. From (2.35), we note that *B*, *A* and b_j for $j = 1(1)K$ are parameters that may contain approximations of $y\left(x_n\right)$ and higher derivatives of $y\left(x_n\right)$. Ikhile (2001) gave some examples of (2.35) for different values of *K*. For $K = 1$, (2.35) becomes

$$y_{n+1} = y_n + \frac{2h\left(y_n'\right)^2}{2y_n' - hy_n''}, \tag{2.36}$$

which is a second order method. Notice that (2.36) is identical to (2.25) and (2.29). For $K=2$, (2.35) becomes

$$y_{n+1}=y_n+\frac{12h\left(y_n'\right)^3}{12\left(y_n'\right)^2-6hy_n'y_n''-2h^2y_n'y_n'''+3h^2\left(y_n''\right)^2}, \tag{2.37}$$

which is a third order method. Ikhile (2001) had claimed that

$$y_{n+1}=y_n+\frac{hy_n'}{1+\sum_{j=1}^{K}b_jx_{n+1}^j} \tag{2.38}$$

is the equivalent formulation of (2.35). Ikhile (2001) had revealed that (2.36) and (2.37) are quite impressive when solving (2.1) whose solutions possess singularities.

Ikhile (2002) gave a more general rational interpolant compare to (2.30) which is given by

$$y(x)\approx Q_m(x)+\frac{x^{m+1}P_{k-s}(x)}{1+\sum_{j=1}^{k}b_jx^j}, \tag{2.39}$$

where

$$Q_m(x)=\sum_{j=0}^{m}d_jx^j, \tag{2.40}$$

$$P_{k-s}(x)=\sum_{j=0}^{k-s}a_jx^j, \tag{2.41}$$

for $k\geq 1,\ s\geq 1,\ m\geq 0,\ s\geq m+1,\ k-s\geq 0$. Based on the interpolant in (2.39), Ikhile (2002) had considered the one-step rational method as

$$y_{n+1}=Q_m(x_{n+1})+\frac{x_{n+1}^{m+1}P_{k-s}(x_{n+1})}{1+\sum_{j=1}^{k}b_jx_{n+1}^j}, \tag{2.42}$$

where

$$Q_m(x_{n+1}) = \sum_{j=0}^{m} d_j x_{n+1}^j, \quad (2.43)$$

$$P_{k-s}(x_{n+1}) = \sum_{j=0}^{k-s} a_j x_{n+1}^j, \quad (2.44)$$

with $k \geq 1$, $s \geq 1$, $m \geq 0$, $s \geq m+1$, $k-s \geq 0$, for the initial value problem (2.1). We note that y_{n+1} and $y(x_{n+1})$ are the numerical and theoretical solutions of (2.1) respectively. From (2.42), (2.43) and (2.44), we note that b_j for $j=1(1)k$; d_j for $j=0(1)m$ and a_j for $j=0(1)(k-s)$ are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$. Ikhile (2002) had shown that the attainable order of the method (2.42) is $m+2k-s+1$. According to Ikhile (2002), (2.42) with $k=s=1$ and $m \geq 0$ yields the rational methods given by (2.13). For $k=s=1$ and $m=0$, Ikhile (2002) had obtained the method given by (2.36) and used it as a basic integrator to form a polynomial extrapolation scheme and a rational extrapolation scheme. According to Ikhile (2002), the rational extrapolation scheme is more accurate than the polynomial extrapolation scheme in solving a problem whose solution possesses singularity.

Ikhile (2004) had showed a class of one-step rational methods given in the form of

$$y_{n+1} = \frac{y_n}{1+\sum_{j=1}^{k} b_j x_{n+1}^j}, \ k \geq 1, \quad (2.45)$$

where b_j for $j=1(1)k$ are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$. The process of obtaining the method is by matching with its Taylor's series, and solve for the parameters b_j for $j=1(1)k$. According to

Ikhile (2004), the order of (2.45) is equals to *k*. For $k=1$, (2.45) reduces to (2.18) while for $k=2$, the following method is obtained

$$y_{n+1}=\frac{2y_n^{\ 3}}{2y_n^{\ 2}-2hy_ny_n'-h^2\left(y_ny_n''-2\left(y_n'\right)^2\right)}. \tag{2.46}$$

Next, methods (2.36) and (2.46) were used as basic integrators to form two polynomial extrapolation schemes and two rational extrapolation schemes. According to Ikhile (2004), (2.46) has perform better than (2.36) in both polynomial and rational extrapolation schemes in solving a problem whose solution possesses singularity.

Ramos (2007) came out with a new approximation algorithm, which according to Ramos (2007), was inspired by the work of Van Niekerk (1987). Ramos (2007) had suggested an approximation to the theoretical solution $y\left(x_{n+1}\right)$ of (2.1) given by

$$y\left(x_{n+1}\right)=y\left(x_n+h\right)=y\left(x_n\right)+\frac{hy'\left(x_n\right)}{a\left(h\right)+y\left(x_n\right)} \tag{2.47}$$

where $a\left(h\right)$ is sufficiently differentiable unknown function of the step-size that has to be determined and it is assume that $a\left(h\right)+y\left(x_n\right)\neq 0$. Ramos (2007) gave the final integration formula which is a second order and *A*-stable method as

$$y_{n+1}=y_n+\frac{2h\left(y_n'\right)^2}{2y_n'-hy_n''}. \tag{2.48}$$

The method (2.48) is identical to (2.25) of Van Niekerk (1987), (2.29) of Van Niekerk (1988) and (2.36) of Ikhile (2001). The local truncation error of (2.48) is given by

$$T_{n+1}=h^3\left(-\frac{\left(y''\left(x_n\right)\right)^2}{4y'\left(x_n\right)}+\frac{y'''\left(x_n\right)}{6}\right)+O\left(h^4\right),$$

where $y'(x_n)$, $y''(x_n)$ and $y'''(x_n)$ denote the first, second and third derivatives of the theoretical solution $y(x_n)$ respectively. Method (2.48) has been tested on a stiff problem, a stiff system, a singular perturbed problem and an autonomous problem. Numerical results had shown that method (2.48) performs very well when solving these problems.

Okosun & Ademiluyi (2007a), and Okosun & Ademiluyi (2007b) had proposed a class of *k*-step rational methods that are based on the same generalization of the *k*-step rational methods of Fatunla (1982) given by (2.23), but with a_r for $r = 1(1)k$ are parameters that may contain approximations of $y(x_n)$ and higher derivatives of $y(x_n)$. It is important to note that the process of obtaining the schemes as shown in Okosun & Ademiluyi (2007a), and Okosun & Ademiluyi (2007b) is by matching with its Taylor series. This approach is very different from that of Fatunla (1982) which interpolates the known values y_n and y'_n at previously computed points (Ikhile, 2004). According to their articles, the resulting 2-step second order method and 3-step third order method are

$$y_{n+2} = \frac{2y_n{}^3}{2y_n{}^2 - 2hy_ny'_n + h^2\left(2\left(y'_n\right)^2 - y_ny''_n\right)} \tag{2.49}$$

and

$$y_{n+3} = \frac{6y_n{}^4}{6y_n{}^3 - 6hy'_ny_n{}^2 + 3h^2y_n\left(2\left(y'_n\right)^2 - y_ny''_n\right) - h^3\left(6\left(y'_n\right)^3 - 6y_ny'_ny''_n + y_n{}^2y'''_n\right)} \tag{2.50}$$

respectively. However, our reviews and inspections reveal that methods (2.49) and (2.50) are incorrect due to the mistakes made in the process of derivations as shown in Okosun & Ademiluyi (2007a), and Okosun & Ademiluyi (2007b). Hence, we make some corrections to the works of Okosun & Ademiluyi (2007a), and Okosun & Ademiluyi (2007b) by presenting the correct 2-step schemes and 3-step schemes as shown below:

$$y_{n+2} = \frac{{y_n}^3}{{y_n}^2 - 2hy_n y_n' + h^2\left(4\left(y_n'\right)^2 - 2y_n y_n''\right)} \tag{2.51}$$

and

$$y_{n+3} = \frac{2{y_n}^4}{2{y_n}^3 - 6hy_n'{y_n}^2 + 9h^2 y_n\left(2\left(y_n'\right)^2 - y_n y_n''\right) - 9h^3\left(6\left(y_n'\right)^3 - 6y_n y_n' y_n'' + {y_n}^2 y_n'''\right)} \tag{2.52}$$

respectively. Numerical results shown in Okosun & Ademiluyi (2007a), and Okosun & Ademiluyi (2007b) had confirmed the suitability of these methods in solving problem whose solution possesses singularity.

On adopting the idea of Okosun & Ademiluyi (2007a) and Okosun & Ademiluyi (2007b), Yaacob *et al*. (2010), Teh *et al.* (2011) and Teh & Yaacob (2013a) have came out with three different classes of 2-step rational methods. For the ease of discussion, rational methods in multistep setting are generally called rational multistep methods (RMMs). Yaacob *et al.* (2010) chose to modify the interpolant (2.12) by changing the interval of integration from $\left[x_n, x_{n+1}\right]$ to $\left[x_n, x_{n+2}\right]$. This yields a class of 2-step *p*-th order rational methods known as RMM1(2,*p*), which can be expressed as follows:

$$y_{n+2} = \frac{\sum_{j=0}^{k} a_j h^j}{b+h},\ k \geq 1,\ b+h \neq 0, \tag{2.53}$$

where b and a_j for $j = 0,1,\ldots,k$ are parameters that may contain $y\left(x_n\right)$ and higher derivatives of $y\left(x_n\right)$. By doing the same modifications to the interval of integration of interpolants (2.27) and (2.35), the following 2-step rational methods can be attained:

$$y_{n+2} = a_0 + \cfrac{a_1 h}{1 + \cfrac{a_2 h}{1 + \cfrac{a_3 h}{1 + \cdots \atop \vdots \atop \cfrac{a_k h}{1 + a_{k+1} h}}}}, \ k \geq 1, \ 1 + a_{k+1} h \neq 0, \tag{2.54}$$

and

$$y_{n+2} = B + \frac{Ah}{1 + \sum_{j=1}^{K} b_j h^j}, \ K \geq 1, \ 1 + \sum_{j=1}^{K} b_j h^j \neq 0, \tag{2.55}$$

respectively. Formula (2.54) belongs to a class of 2-step p-th order rational methods, known to be RMM2(2,p) in Teh *et al.* (2011). On the other hand, Teh & Yaacob (2013a) considered another class of 2-step p-th order rational methods based on the formula (2.55), or better known as RMM3(2,p).

RMMs of order 2 until order 5 were derived for each class of RMM i.e. RMM1(2,p), RMM2(2,p) and RMM3(2,p). Absolute stability analysis for each derived method is carried out and a comparison in the sense of L-stability and A-stability can be shown in Table 2.1.

Table 2.1: Stability Analyses of 2-step RMMs

Order (*p*)	**RMM1(2,*p*)**	**RMM2(2,p)**	**RMM3(2,p)**
2	*A*-stable	*A*-stable	*A*-stable
3	Not *A*-stable	Not *A*-stable	*A*-stable
4	Not *A*-stable	*A*-stable	*A*-stable
5	Not *A*-stable	Not *A*-stable	Not *A*-stable

From Table 2.1, we can see that there is no *L*-stable method in either RMM1(2,*p*), RMM2(2,*p*) or RMM3(2,*p*). In general, numerical comparison among RMM1(2,*p*), RMM2(2,*p*) and RMM3(2,*p*) showed that: RMM3(2,*p*) outperform RMM2(2,*p*) and RMM1(2, *p*) when solving scalar initial value problems including problem whose solutions possesses singularity; and when solving initial value problem with system of ordinary differential equations, all three classes of RMMs have comparable accuracy. Therefore, the strength of RMM3(2,*p*) becomes apparent when solving scalar initial value problems (Teh & Yaacob, 2013a). In addition, RMM1(2,*p*), RMM2(2,*p*) and RMM3(2,*p*) are more accurate than the RMMs proposed by Okosun & Ademiluyi (2007a) and Okosun & Ademiluyi (2007b) (Yaacob *et al.*, 2010; Teh *et al.*, 2011; Teh & Yaacob, 2013a).

Yaacob *et al.* (2010), Teh *et al.* (2011) and Teh & Yaacob (2013a) have showed that generalizations to *r*-step *p*-th order RMM1, RMM2 and RMM3 are possible. This can be achieved by simply extending the interval of integration from $\left[x_n, x_{n+2}\right]$ to $\left[x_n, x_{n+r}\right]$ on the interpolants (2.12), (2.27) and (2.35). Hence, RMM1(*r*,*p*) (read as *r*-step *p*-th order RMM1), RMM2(*r*,*p*) and RMM3(*r*,*p*) are given by

$$y_{n+r} = \frac{\sum_{j=0}^{k} a_j h^j}{b+h}, \; k \geq 1, \; b+h \neq 0; \tag{2.56}$$

$$y_{n+r} = a_0 + \cfrac{a_1 h}{1+\cfrac{a_2 h}{1+\cfrac{a_3 h}{1+\cdots}}}, \; k \geq 1, \; 1+a_{k+1}h \neq 0; \tag{2.57}$$

$$\vdots$$

$$\frac{a_k h}{1+a_{k+1}h}$$

and

$$y_{n+r} = B + \frac{Ah}{1+\sum_{j=1}^{K} b_j h^j}, \; K \geq 1, \; 1+\sum_{j=1}^{K} b_j h^j \neq 0, \tag{2.58}$$

respectively. We note that these three extended classes of RMMs are variable order methods that are independent of the step number r. However, at this moment, there are no numerical experimentations being carried out to verify the efficiency of the formulae (2.56), (2.57) and (2.58).

Teh *et al.* (2009) and Teh (2010) have made a collective review on several classes of one-step rational methods proposed by Lambert & Shaw (1965), Van Niekerk (1987), Van Niekerk (1988) and Ramos (2007). Existing rational methods of order 2 until order 5 were derived and comparisons in terms of absolute stability and numerical accuracy were carried out. Table 2.2 showed the stability analyses in the sense of A-stability and L-stability for the methods mentioned in this paragraph.

Table 2.2: Stability Analyses of Several Existing One-step Rational Methods

Order	**Lambert & Shaw (1965)**	**Van Niekerk (1987)**	**Van Niekerk (1988)**	**Ramos (2007)**
2	*A*-stable	*A*-stable	*A*-stable	*A*-stable
3	Not *A*-stable	*L*-stable	Not *A*-stable	*A*-stable
4	Not *A*-stable	*A*-stable	*A*-stable	*A*-stable
5	Not *A*-stable	*L*-stable	Not *A*-stable	Not *A*-stable

Findings from Teh *et al.* (2009) and Teh (2010) showed that all existing rational methods by Lambert & Shaw (1965), Van Niekerk (1987), Van Niekerk (1988) and Ramos (2007) are suitable in solving a variety of initial value problems such as stiff problem and problem whose solution possesses singularity. However, rational methods that are *L*-stable or *A*-stable are more preferable when solving stiff problem. According to Teh *et al.* (2009) and Teh (2010), rational methods from Van Niekerk (1987) are the most suitable to solve stiff problems; followed by rational methods from Van Niekerk (1988). Rational methods given by Lambert & Shaw (1965) can be used to solve stiff problem if the step-size of integration is sufficiently small. Rational methods given by Lambert & Shaw (1965) still produce good results under this restriction, particularly for explicit methods. Furthermore, rational methods from Lambert & Shaw (1965) are the cheapest algorithms to implement. As for the rational methods based on interpolant (2.47) by Ramos (2007), they do not perform as good as those rational methods given by Van Niekerk (1987) and Van Niekerk (1988). However, when solving problem whose solution possess singularity, rational methods from Ramos (2007) are the most suitable and most accurate.

Stability issue arises from the implementation of numerical method to stiff problem is always a great concern when developing numerical method for initial value problem. Therefore, *L*-stability or *A*-stability in a numerical method is desirable or even better if *L*-stability or *A*-stability is guaranteed. From our readings of previous works including the works by Teh *et al.* (2009) and Teh (2010), the stability conditions of a particular class of rational methods are affected by the underlying rational functions (or interpolants). All existing rational methods mentioned earlier were based on conventional rational functions. If these existing rational methods are applied to the scalar test problem given in (1.2), then none of them give an exact solution to the test problem (1.2) (Teh & Yaacob, 2013b). In other words, none of the existing rational method is exponentially-fitted. There are two advantages for a numerical method being exponentially-fitted: firstly, it returns the exact solution to the test problem (1.2) and secondly, *L*-stability is guaranteed (Wu, 1998).

To develop exponential-fitted rational methods, conventional rational functions (or interpolants) such as (2.12), (2.15), (2.19), (2.23), (2.27), (2.32), (2.35), (2.42), (2.45) or (2.47) need to be modified. An example of such modification was done by Teh (2010) and Teh & Yaacob (2013b) when they suggested the following approximation to the theoretical solution of (2.1) by the formula

$$y_{n+1} = \frac{\sum_{i=0}^{k} a_i h^i + c_1 e^{c_2 h}}{1+bh}, \; 1+bh \neq 0, \tag{2.59}$$

where b, c_1, c_2 and a_i for $i = 0,1,\ldots,k$ are parameters that may contain $y(x_n)$ and higher derivatives of $y(x_n)$. We have observed that the numerator of formula (2.59) is the composition of a polynomial and an exponential function, while the denominator is a polynomial of degree 1. According to Teh (2010) and Teh &

Yaacob (2013b), formula (2.59) is known as one-step exponential-rational method (in brief as ERM). If an ERM has order p, then this particular ERM is noted as p-ERM. ERMs of order 2 until order 5 were developed and discussed in Teh (2010) and Teh & Yaacob (2013b); and all of them are proved to be L-stable. Findings from Teh (2010) and Teh & Yaacob (2013b) had showed that the capability of ERMs in solving problem whose solution possesses singularity is less obvious but in return, ERMs are more reliable in solving general initial value problems including non-stiff and stiff problems.

Despite ERMs' strong stability characteristics and better accuracies, they have two shortcomings which could be observed from the findings of Teh (2010) and Teh & Yaacob (2013b). First, from the process of derivations, one must have noticed that the parameter c_2 of a p-ERM in (2.59) is not unique. In other words, a p-ERM is not unique but two different methods which share the same order of accuracy. Secondly, the parameter c_2 of every p-ERM contains expression with square root. In other words, there are times where an ERM will produce numerical solutions that are complex numbers due to the square root evaluations. These two disadvantages of ERMs become the main rationales of this new study, where we wish to modify the original ERMs in (2.59), so that the newly modified ERMs are free from the two defects mentioned above. The developments and implementations of the new modified ERMs will be presented in Chapter 3.

Last but not least, all ERMs as well as most of the existing rational methods are implemented using constant step-size where error estimation at each integration step is neglected. However, there are two exceptions. Both Ikhile (2002) and Ikhile (2004) considered variable step-size strategies in extrapolation methods. The difference between these two papers is: formula (2.36) becomes the basic integrator in Ikhile (2002) while formula (2.46) becomes the basic integrator for Ikhile (2004). Findings from both papers showed that extrapolation methods with step-size control are more accurate than those extrapolation methods with constant step-size especially in solving problem whose solution possesses singularity. Perhaps with the variation in the step-size, the numerical results of ERMs may be improved when solving problem (1.1) whose solution possesses singularity. In view of this, a strategy of variation in step-size for the newly modified ERMs and other existing one-step rational methods will be considered. Further discussions on this topic will be presented in Chapter 4.

2.4 Conclusions

In this chapter, we have done some literature reviews for the up-coming studies in this report, where we have clearly stated out the areas of research that have not been explored. We are ready to study them in the following chapters.

CHAPTER THREE

ONE-STEP MODIFIED EXPONENTIAL-RATIONAL METHODS

3.1 Introduction

In this chapter, we shall derive an explicit one-step modified exponential-rational method with generalized parameters. We shall present and explain the process of derivations, as well as its generalized local truncation error and stability function analysis. Consistency and convergence properties of the one-step modified exponential-rational method will be discussed as well. Last but not least, we shall test our newly developed method using some test problems.

3.2 Preliminaries

We are considering the initial value problem

$$y' = f\left(x, y\right), \; y\left(a\right) = \eta ,$$

$$y\,, \; f\left(x, y\right) \in \mathbb{R}\,, \; x \in \left[a, b\right] \subset \mathbb{R}\,, \tag{3.1}$$

where f is assumed to satisfy all the conditions in order that (3.1) has a unique solution. The interval $\left[a, b\right]$ is divided into a number of subintervals $\left[x_n, x_{n+1}\right]$ with $x_0 = a$ and $x_n = x_0 + nh$, such that h is the step-size. Suppose that we have solved numerically the initial value problem in (3.1) up to a point x_n and have obtained a value y_n as an approximation of $y\left(x_n\right)$, which is the theoretical solution of (3.1). From Lambert (1973) and Lambert (1991), assuming the localizing assumption that no previous truncation errors have been made, i.e. $y_n = y\left(x_n\right)$, we are interested in obtaining y_{n+1} as the approximation of $y\left(x_{n+1}\right)$. For that purpose, we suggest an approximation to the theoretical solution $y\left(x_{n+1}\right)$ of (3.1) given by

$$y_{n+1}=\frac{\sum_{j=0}^{k} a_j h^j + c e^{\frac{h y_n'}{y_n}}}{1+bh},\ 1+bh\neq 0,\ k=0,1,2,\ldots, \tag{3.2}$$

where b, c and a_j for $j=0,1,\ldots,k$ are parameters that may contain $y\left(x_n\right)$ and higher derivatives of $y\left(x_n\right)$ and h is the step-size. In view of this, these parameters have to be determined during the derivation process. The value k presented in (3.2) decides the number of derivatives to be evaluated in (3.2) i.e. a total of $y^{(m)}\left(x_n\right)$ for $m=1,2,\ldots,k+2$. The higher the value of k, the more derivatives evaluations need to be carried out.

Formula (3.2) is the modified version of the original exponential-rational method shown in formula (2.59). One has noticed that the exponential functions in both (3.2) and (2.59) are different. Hence, we regard (3.2) as one-step modified exponential-rational method, or in brief as MERM. If a MERM has order p, then this particular MERM is called a p-MERM. With the p-MERM in (3.2), we associate a difference operator L defined by

$$L\left[y(x);h\right]_{p-\text{MERM}}=y\left(x+h\right)\times\left(1+bh\right)-\sum_{j=0}^{k} a_j h^j - c e^{\frac{h y'(x)}{y(x)}},\ k\geq 0,\ p\geq 2, \tag{3.3}$$

where $y\left(x\right)$ is an arbitrary function, continuously differentiable on $x\in\left[a,b\right]\subset\mathbb{R}$. Expanding $y\left(x+h\right)$ and exponential function $e^{hy'(x)/y(x)}$ as Taylor series, and collecting terms in (3.3) gives the following general expression:

$$L\left[y(x);h\right]_{p-\text{MERM}}=C_0h^0+C_1h^1+\cdots+C_kh^k+C_{k+1}h^{k+1}+C_{k+2}h^{k+2}+\cdots. \tag{3.4}$$

We note that C_i, $i = 0,1,2,\ldots$ in (3.4) contains corresponding parameters that need to be determined in the derivation processes. To facilitate the derivation of MERM, the order and local truncation error of *p*-MERM are defined as follows.

Definition 3.1 *The difference operator (3.3) and the associated modified exponential-rational method (3.2) is said to be of order* $p = k + 2$ *if, in (3.4),* $C_0 = C_1 = C_2 = \cdots = C_{k+2} = 0$, $C_{k+3} \neq 0$ *for* $k = 0,1,2,\ldots$.

Definition 3.2 *The local truncation error at* x_{n+1} *of (3.2) is defined to be the expression* $L\left[y\left(x_n\right);h\right]_{p-\mathrm{MERM}}$ *given by (3.3), when* $y\left(x_n\right)$ *is the theoretical solution of the initial value problem (3.1) at a point* x_n. *The local truncation error of (3.2) is then*

$$L\left[y\left(x_n\right);h\right]_{p-\mathrm{MERM}} = C_{k+3}h^{k+3} + O\left(h^{k+4}\right). \tag{3.5}$$

From Definition 3.1, it is important to note that

$$k = p - 2, \tag{3.6}$$

since we are going to use this expression in the remainder of this chapter.

3.3 Derivation of One-step Modified Exponential-Rational Method

The derivation of one-step MERM is all about finding the unknown coefficients (parameters) *b*, *c* and a_j for $j = 0,1,\ldots,k$ in formula (3.2). First, we must determine the desired order accuracy by setting an arbitrary value for *p*. Then, the value of *k* can be obtained once the arbitrary value of *p* is determined using the equation (3.6). Next, from (3.3), we have to expand $y(x+h)$ and $e^{hy'(x)/y(x)}$ as Taylor series and also expand the polynomial $\sum_{j=0}^{k} a_j h^j$ up to degree *k*. After that, we must arrange the expanded (3.3) until equation (3.4) is achieved. Upon comparison between the expanded (3.3) and (3.4), we can identify the expressions which correspond to C_0, C_1, …, C_{k+2} and C_{k+3}. Finally, with $C_0 = C_1 = \cdots = C_{k+2} = 0$, and taking $y(x)$ as the theoretical solution of the initial value problem (3.1) i.e. $y(x) = y(x_n)$, we can obtain a system of $k+2$ simultaneous equations as shown below:

$$\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \frac{-y_n}{0!} & \frac{y_n'}{1!\,y_n} \\
0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \frac{-y_n'}{1!} & \frac{(y_n')^2}{2!(y_n)^2} \\
0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & \frac{-y_n''}{2!} & \frac{(y_n')^3}{3!(y_n)^3} \\
0 & 0 & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & \frac{-y_n'''}{3!} & \frac{(y_n')^4}{4!(y_n)^4} \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 0 & \frac{-y_n^{(p-5)}}{(p-5)!} & \frac{(y_n')^{p-4}}{(p-4)!(y_n)^{p-4}} \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 0 & \frac{-y_n^{(p-4)}}{(p-4)!} & \frac{(y_n')^{p-3}}{(p-3)!(y_n)^{p-3}} \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & \frac{-y_n^{(p-3)}}{(p-3)!} & \frac{(y_n')^{p-2}}{(p-2)!(y_n)^{p-2}} \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \frac{-y_n^{(p-2)}}{(p-2)!} & \frac{(y_n')^{p-1}}{(p-1)!(y_n)^{p-1}} \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \frac{-y_n^{(p-1)}}{(p-1)!} & \frac{(y_n')^{p}}{p!(y_n)^{p}}
\end{pmatrix}
\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ \vdots \\ a_{p-4} \\ a_{p-3} \\ a_{p-2} \\ b \\ c \end{pmatrix}
=
\begin{pmatrix} \frac{y_n}{0!} \\ \frac{y_n'}{1!} \\ \frac{y_n''}{2!} \\ \frac{y_n'''}{3!} \\ \frac{y_n^{(4)}}{4!} \\ \vdots \\ \frac{y_n^{(p-4)}}{(p-4)!} \\ \frac{y_n^{(p-3)}}{(p-3)!} \\ \frac{y_n^{(p-2)}}{(p-2)!} \\ \frac{y_n^{(p-1)}}{(p-1)!} \\ \frac{y_n^{(p)}}{p!} \end{pmatrix}. \tag{3.7}$$

The system of equations in (3.7) is used to determine the unknown coefficients b, c and a_j for $j = 0,1,\ldots,k$. These coefficients, in fact, facilitate a generalization of MERMs of arbitrary order *p*. In other words, the coefficients can be computed once the desired order of accuracy (*p*) is determined.

On solving the system (3.7) for the unknown coefficients b, c and a_j for $j = 0,1,\ldots,k$ using *MATHEMATICA 8.0* software, we obtain the following generalized formulae:

$$a_0 = y_n + \frac{(y_n)^p (y_n')^{1-p}\left[(p-2)!\,p!\left(y_n^{(p-1)}\right)^2 - \left((p-1)!\right)^2 y_n^{(p-2)} y_n^{(p)}\right]}{\left((p-1)!\right)^2 y_n' y_n^{(p-2)} - (p-2)!\,p!\,y_n y_n^{(p-1)}}, \tag{3.8}$$

$$\begin{aligned} a_j = {} & (y_n)^{-j} (y_n')^{-p}\Big[-j!(p-2)!(p-1)!(y_n)^j (y_n')^{p+1} y_n^{(j-1)} y_n^{(p-1)} \\ & + j!(p-2)!(p-1)!(y_n)^{j+1} (y_n')^p y_n^{(j-1)} y_n^{(p)} \\ & + (j-1)!(y_n)^p (y_n')^{j+1}\left((p-2)!\,p!\left(y_n^{(p-1)}\right)^2 - \left((p-1)!\right)^2 p!\,y_n^{(p-2)} y_n^{(p)}\right)\Big] \Big/ \\ & \left((j-1)!\,j!\left[\left((p-1)!\right)^2 y_n' y_n^{(p-2)} - (p-2)!\,p!\,y_n y_n^{(p-1)}\right]\right), \end{aligned} \tag{3.9}$$

$$b = \frac{(p-2)!(p-1)!\left(y_n' y_n^{(p-1)} - y_n y_n^{(p)}\right)}{-\left((p-1)!\right)^2 y_n' y_n^{(p-2)} + (p-2)!\,p!\,y_n y_n^{(p-1)}}, \tag{3.10}$$

and

$$c = -\frac{(y_n)^p (y_n')^{1-p}\left[(p-2)!\,p!\left(y_n^{(p-1)}\right)^2 - \left((p-1)!\right)^2 y_n^{(p-2)} y_n^{(p)}\right]}{\left((p-1)!\right)^2 y_n' y_n^{(p-2)} - (p-2)!\,p!\,y_n y_n^{(p-1)}}, \tag{3.11}$$

where $y_n = y(x_n)$ and $y_n^{(m)} = y^{(m)}(x_n)$ for $j = 1,2,\ldots,k$, $p = k+2$ and $m = 1,2,\ldots,p$ by the localizing assumption. We note that formulae (3.2) and (3.8) – (3.11) are valid provided that $y_n = y(x_n) \neq 0$.

3.4 Local Truncation Error of Modified Exponential-Rational Method

In the process of identifying the expressions which correspond to C_0, C_1, …, C_{k+2} and C_{k+3} and taking $y(x)$ as the theoretical solution of the initial value problem (3.1) i.e. $y(x)=y(x_n)$, we found that

$$C_{k+3}=-\frac{c\left(y_n'\right)^{p+1}}{(p+1)!\left(y_n\right)^{p+1}}+\frac{by_n^{(p)}}{p!}+\frac{y_n^{(p+1)}}{(p+1)!}, \tag{3.12}$$

for arbitrary value of *p* (or arbitrary value of *k*). Therefore, from Definition 3.2, the local truncation error (in brief as LTE) of a *p*-MERM (3.2) is given by

$$\mathrm{LTE}_{p-\mathrm{MERM}}=h^{p+1}\left(-\frac{c\left(y_n'\right)^{p+1}}{(p+1)!\left(y_n\right)^{p+1}}+\frac{by_n^{(p)}}{p!}+\frac{y_n^{(p+1)}}{(p+1)!}\right)+O\left(h^{p+2}\right), \tag{3.13}$$

where $y_n=y(x_n)$, $y_n'=y'(x_n)$, $y_n^{(p)}=y^{(p)}(x_n)$ and $y_n^{(p+1)}=y^{(p+1)}(x_n)$ by the localizing assumption. We note that the LTE formula (3.13) is valid provided that $y_n=y(x_n)\neq 0$. The parameters *b* and *c* in formula (3.13) are determined from the formulae (3.10) and (3.11), respectively.

3.5 Absolute Stability Analysis of Modified Exponential-Rational Method

The absolute stability analysis of a *p*-MERM can be obtained easily by applying the formulae (3.2) and (3.8) – (3.11) to the Dahlquist's test equation:

$$y'=\lambda y,\ y(a)=y_0,\ \lambda\in\mathbb{C},\ \mathrm{Re}(\lambda)<0. \tag{3.14}$$

It can be shown that, the application of a *p*-MERM (3.2) to the Dahlquist's test problem resulted in the following difference equation:

$$y_{n+1}=R(z)\,y_n,\ z=h\lambda. \tag{3.15}$$

We note that $R(z)$ is the stability function of a *p*-MERM. Clearly $y_n \to 0$ as $n \to \infty$ if and only if

$$\left|R(z)\right| < 1. \tag{3.16}$$

A *p*-MERM is absolutely stable for those values of *z* for which the condition in (3.16) holds. The region of absolute stability of a *p*-MERM is defined as $\left\{z \in \mathbb{C} : \left|R(z)\right| \le 1\right\}$ or the set of points in the complex plane such that the approximated solution remains bounded after many steps of integrations (Butcher, 2008).

On applying the Dahlquist's test equation (3.14) to formulae (3.8) – (3.11) and simplifying them using *MATHEMATICA* 8.0 software, we arrive at the following results:

$$a_0 = 0,\ a_j = 0,\ b = 0 \text{ and } c = y_n. \tag{3.17}$$

Then, apply the test equation (3.14) to formula (3.2) and also substitute the results in (3.17) into formula (3.2) to yield the followng:

$$\begin{aligned} y_{n+1} &= \frac{\sum_{j=0}^{k} a_j h^j + c e^{\frac{h y_n'}{y_n}}}{1 + bh} \\ &= \frac{a_0 + \sum_{j=1}^{k} a_j h^j + c e^{\frac{h\lambda y_n}{y_n}}}{1 + bh} \\ &= e^{h\lambda} y_n. \end{aligned} \tag{3.18}$$

If we let $z = h\lambda$, then we obtain

$$y_{n+1} = e^z y_n,$$

and according to equation (3.15), the stability function of *p*-MERM is

$$R(z) = e^z. \tag{3.19}$$

In other words, the stability function of MERM for any order of accuracy is always the function given in equation (3.19). On setting $z = x + \mathrm{i}y$, we obtain the region of absolute stability of a *p*-MERM as illustrated in Figure 3.1.

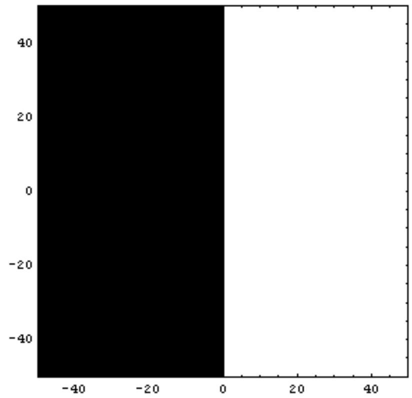

Figure 3.1 Region of absolute stability of a p-MERM

The shaded region in Figure 3.1 is the region of absolute stability of a *p*-MERM, where the condition $|R(z)| \le 1$ is satisfied. From Figure 3.1, we can see that the region of absolute stability of a *p*-MERM contains the whole left-hand half plane, which show that any *p*-th order MERM is *A*-stable. In addition, on using *MATHEMATICA 8.0*, we have found out that $|R(z)| \to 0$ as $\mathrm{Re}(z) \to -\infty$. This shows that any *p*-th order MERM is also *L*-stable.

3.6 Consistency and Convergence Analyses of Modified Exponential-Rational Method

We now show that any *p*-th order MERM is consistent with the differential equation in (3.1) by the following definition.

Definition 3.3 *The MERM (3.2) is said to be consistent if (3.5) satisfy*

$$\lim_{\substack{h\to 0\\ x=a+nh}} \frac{1}{h} L\left[y\left(x_n\right);h\right]_{p-\mathrm{MERM}} = 0. \tag{3.20}$$

From Definition 3.2, $L\left[y\left(x_n\right);h\right]_{p-\mathrm{MERM}}$ is essentially the local truncation error for a p-MERM. It can be shown that the local truncation error for any p-th order MERM satisfy the condition in (3.20), which directly implies any p-th order MERM is consistent with the differential equation in (3.1). Below is a proof which shows that the local truncation error for any p-th order MERM does satisfy the condition in (3.20):

$$\begin{aligned}
&\lim_{\substack{h\to 0\\ x=a+nh}} \frac{1}{h} L\left[y\left(x_n\right);h\right]_{p-\mathrm{MERM}} \\
&= \lim_{\substack{h\to 0\\ x=a+nh}} \frac{1}{h}\left(h^{p+1}\left(-\frac{c\left(y_n'\right)^{p+1}}{(p+1)!\left(y_n\right)^{p+1}} + \frac{by_n^{(p)}}{p!} + \frac{y_n^{(p+1)}}{(p+1)!} \right) + O\left(h^{p+2}\right)\right) \\
&= \lim_{\substack{h\to 0\\ x=a+nh}} h^{p}\left(-\frac{c\left(y_n'\right)^{p+1}}{(p+1)!\left(y_n\right)^{p+1}} + \frac{by_n^{(p)}}{p!} + \frac{y_n^{(p+1)}}{(p+1)!} + O\left(h\right)\right) \\
&= 0.
\end{aligned}$$

Lastly, according to Fatunla (1988), the convergence of a p-MERM can be verified, since its application to the Dahlquist's test equation (3.14) results in the following difference equation:

$$y_n = \left(e^{h\lambda}\right)^n y_0. \tag{3.21}$$

We note that equation (3.21) is derived from equation (3.18). From equation (3.21), since $\left(e^{h\lambda}\right)^n \to 0$ as $n\to\infty$ for all $h\lambda$ with $\mathrm{Re}\left(\lambda\right)<0$, we have $y_n \to 0$ as $n\to\infty$ which, in the limit, does satisfy

$$\lim_{\substack{n\to\infty \\ h\to 0}} y_n = y(x_n). \tag{3.22}$$

This is because the theoretical solution of test equation (3.14) also behaves like $y(x_n)\to 0$ as $n\to\infty$. In other words, both y_n and $y(x_n)$ approach zero as n approaches infinity.

3.7 Numerical Experiments and Comparisons

Theoretically, newly developed MERMs and existing rational methods are effective methods in solving initial value problem (3.1). However, we still need to clarify whether MERMs and existing rational methods can solve the following classes of (3.1):

(a) (3.1) whose initial condition $y(a)=\eta=0$;

(b) (3.1) in non-autonomous form;

(c) (3.1) in autonomous form; and

(d) (3.1) whose solutions possess singularities.

According to Teh (2010), rational methods suggested by Lambert & Shaw (1965), Van Niekerk (1987), Van Niekerk (1988) and Ikhile (2001) face no difficulty in solving initial value problem (3.1) whose initial condition $y(a)=\eta=0$. All ERMs by Teh (2010) are capable to solve (3.1) with initial condition $y(a)=\eta=0$, except for 2-ERM(1) and 2-ERM(2). This is because the parameters c_2 and b for 2-ERM(1) and 2-ERM(2) become undefined if the initial condition is zero. As for the MERMs given by formula (3.2), it is very obvious that a p-th order MERM is not designed to solve initial value problem with initial condition zero because the exponential function will be undefined.

Item (b) and item (c) should not cause any problem to any existing rational method but just to make sure that our new MERMs manage to cope with non-autonomous problem and autonomous problem. Lastly, we want to investigate whether MERMs can solve problem whose solutions possess singularities as stated in item (d). We note that previous researches show that existing rational methods have no difficulty in solving this kind of problem.

For the investigations mentioned above, we choose to compare the third order MERM with existing third order rational methods from Lambert & Shaw (1965), Van Niekerk (1987), Van Niekerk (1988), Ikhile (2001) and Teh & Yaacob (2013b). Third order rational methods are chosen due to simplicity, the requirement of fewer evaluations of higher derivatives and less computational time. Some test problems are used to check the accuracy of these third order rational methods with different number of integration steps. We present the maximum absolute relative errors over the integration interval given by $\max\limits_{0\le n\le N}\left\{\left|y\left(x_n\right)-y_n\right|\right\}$ where N is the number of integration steps. We note that $y\left(x_n\right)$ and y_n represents the theoretical solution and numerical solution of a test problem at point x_n.

We present the third order rational methods that are involved in the following numerical experimentation and comparisons. Firstly, the new third order MERM, or 3-MERM:

$$y_{n+1}=\frac{a_0+a_1h+ce^{\frac{hy'_n}{y_n}}}{1+bh},\ 1+bh\neq 0, \tag{3.23}$$

with

$$\begin{cases} a_0 = y_n - \dfrac{(y_n)^3\left(-3(y_n'')^2 + 2y_n' y_n'''\right)}{(y_n')^2\left(2(y_n')^2 - 3y_n y_n''\right)}, c = \dfrac{(y_n)^3\left(-3(y_n'')^2 + 2y_n' y_n'''\right)}{(y_n')^2\left(2(y_n')^2 - 3y_n y_n''\right)}, \\ a_1 = -\dfrac{-2(y_n')^4 + 4y_n(y_n')^2 y_n'' - 3(y_n)^2(y_n'')^2 + (y_n)^2 y_n' y_n'''}{y_n'\left(2(y_n')^2 - 3y_n y_n''\right)}, b = -\dfrac{y_n' y_n'' - y_n y_n'''}{2(y_n')^2 - 3y_n y_n''} \end{cases}.$$

We note that 3-MERM (3.23) is L-stable as mentioned in Section 3.5. The third order rational method by Lambert & Shaw (1965) is given by

$$y_{n+1} = y_n + hy_n' + \frac{h^2}{2} y_n'' + \frac{h^3}{2} \frac{y_n'' y_n'''}{3y_n'' - hy_n'''}. \tag{3.24}$$

Absolute stability analysis showed that formula (3.24) is not A-stable (Teh, 2010).

The third order rational methods by Van Niekerk (1987) and Van Niekerk (1988) are given by

$$\begin{aligned} y_{n+1} = y_n &+ \frac{hy_n y_n'}{y_n - hy_n'} \\ &+ \frac{3h^2\left(-2(y_n')^2 + y_n y_n''\right)^2}{(-y_n + hy_n')\left(12(y_n')^2 - 6y_n y_n'' - 6hy_n' y_n'' + 3h^2(y_n'')^2 + 2hy_n y_n''' - 2h^2 y_n' y_n'''\right)}, \end{aligned} \tag{3.25}$$

and

$$y_{n+1} = y_n + hy_n' + \frac{h^2}{2} y_n'' + \frac{h^3}{2} \frac{y_n'' y_n'''}{3y_n'' - hy_n'''}, \tag{3.26}$$

respectively. Absolute stability analyses showed that formula (3.25) is L-stable while formula (3.26) is not A-stable (Teh, 2010). From formulae (3.24) and (3.26), we note that the third order rational methods of Lambert & Shaw (1965) and Van Niekerk (1988) are identical. The third order rational methods from Ikhile (2001) is given by

$$y_{n+1} = y_n + \frac{12h(y_n')^3}{12(y_n')^2 - 6hy_n' y_n'' + h^2\left[3(y_n'')^2 - 2y_n' y_n'''\right]}. \tag{3.27}$$

Absolute stability analysis showed that formula (3.27) is A-stable (Teh, 2010).

Lastly, the two third order exponential-rational methods (ERMs) from Teh & Yaacob (2013b) denoted by 3-ERM(1) and 3-ERM(2) are:

$$y_{n+1} = \frac{a_0 + c_1 e^{c_2 h}}{1+bh},\ 1+bh \neq 0, \tag{3.28}$$

with

$$\left\{ a_0 = y_n - \frac{-2\left(y_n'\right)^2 + y_n y_n''}{c_2\left(c_2 y_n - 2y_n'\right)}, b = \frac{c_2 y_n' - y_n''}{-c_2 y_n + 2y_n'}, c_1 = \frac{-2\left(y_n'\right)^2 + y_n y_n''}{c_2\left(c_2 y_n - 2y_n'\right)}, \right.$$
$$\left. c_2 = \frac{-3y_n' y_n'' + y_n y_n''' - U_2}{2\left(-2\left(y_n'\right)^2 + y_n y_n''\right)} \right\};$$

and

$$y_{n+1} = \frac{a_0 + c_1 e^{c_2 h}}{1+bh},\ 1+bh \neq 0, \tag{3.29}$$

with

$$\left\{ a_0 = y_n - \frac{-2\left(y_n'\right)^2 + y_n y_n''}{c_2\left(c_2 y_n - 2y_n'\right)}, b = \frac{c_2 y_n' - y_n''}{-c_2 y_n + 2y_n'}, c_1 = \frac{-2\left(y_n'\right)^2 + y_n y_n''}{c_2\left(c_2 y_n - 2y_n'\right)}, \right.$$
$$\left. c_2 = \frac{-3y_n' y_n'' + y_n y_n''' + U_2}{2\left(-2\left(y_n'\right)^2 + y_n y_n''\right)} \right\},$$

respectively. We note that

$$U_2 = \sqrt{\left(3y_n' y_n'' - y_n y_n'''\right)^2 - 4\left(-2\left(y_n'\right)^2 + y_n y_n''\right)\left(-3\left(y_n''\right)^2 + 2y_n' y_n'''\right)}.$$

Absolute stability analysis showed formulae (3.28) and (3.29) are *L*-stable (Teh & Yaacob, 2013b).

Problem 3.1

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

The theoretical solution is $y(x) = 4e^{-2x} - 1 + 2x$. *Problem 3.1* is a non-stiff differential equation, and also a non-autonomous problem.

Problem 3.2 (Fatunla, 1982)

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

The theoretical solution is $y(x) = 10 - 10e^{-x} - xe^{-x} + 10e^{-200x}$. *Problem 3.2* is stiff differential equation, and also a non-autonomous problem.

Problem 3.3 (Ramos, 2007)

$$y_1'(x) = -1002y_1(x) + 1000y_2(x)^2,\ y_1(0) = 1,\ x \in [0, 1];$$

$$y_2'(x) = y_1(x) - y_2(x)\left(1 + y_2(x)\right),\ y_2(0) = 1,\ x \in [0, 1];$$

The theoretical solutions are $y_1(x) = e^{-2x}$ and $y_2(x) = e^{-x}$. *Problem 3.3* is a stiff system, and also an autonomous problem.

Problem 3.4 (Yaakub and Evans, 2003)

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

The theoretical solution is $y(x) = 0.01e^{-100x} + e^{-x}$. *Problem 3.4* 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 $y_2(x) = -e^{-100x} - e^{-x}$. *Problem 3.4* is a stiff system, and also an autonomous problem.

Problem 3.5 (Ramos, 2007)

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

The theoretical solution is $y(x) = \tan(x + \pi/4)$. *Problem 3.5* is an example of problem whose solution possesses singularity. From the theoretical solution, notice that the solution becomes unbounded in the neighbourhood of the singularity at $x = \pi/4 \approx 0.785398163367448$.

Table 3.1: Maximum Absolute Relative Errors of Various Third Order Methods with respect to the Number of Steps (Problem 3.1)

N	**Lambert & Shaw (1965)**	**Van Niekerk (1987)**	**Van Niekerk (1988)**	**Ikhile (2001)**	**3-ERM(1)**	**3-ERM(2)**	**3-MERM**
16	5.07503(-06)	3.25864(-04)	5.07503(-06)	5.84945(-05)	-	-	4.24138(-07)
32	6.28976(-07)	2.93414(-05)	6.28976(-07)	7.85013(-06)	-	-	5.28343(-08)
64	7.82908(-08)	3.83339(-06)	7.82908(-08)	1.01742(-06)	-	-	6.58942(-09)

Table 3.2: Maximum Absolute Relative Errors of Various Third Order Methods with respect to the Number of Steps (Problem 3.2)

N	**Lambert & Shaw (1965)**	**Van Niekerk (1987)**	**Van Niekerk (1988)**	**Ikhile (2001)**	**3-ERM(1)**	**3-ERM(2)**	**3-MERM**
100	7.08987(+01)	1.51505(+00)	7.08987(+01)	4.71235(+00)	8.05125(-01)	8.05075(-01)	2.51013(-02)
1000	7.48249(-01)	3.57558(-01)	7.48249(-01)	6.24419(-02)	2.36491(-02)	1.43271(-01)	8.52263(-03)
10000	1.06282(-03)	1.44188(-03)	1.06282(-03)	1.34363(-03)	2.76633(-05)	1.93116(-04)	2.67342(-05)
100000	1.10728(-06)	1.89317(-06)	1.10728(-06)	1.44295(-05)	2.86579(-08)	6.40614(-07)	3.33494(-08)

Table 3.3: Maximum Absolute Relative Errors of Various Third Order Methods with respect to the Number of Steps $(y_1(x))$ *(Problem 3.3)*

N	**Lambert & Shaw (1965)**	**Van Niekerk (1987)**	**Van Niekerk (1988)**	**Ikhile (2001)**	**3-ERM(1)**	**3-ERM(2)**	**3-MERM**
160	2.19212(+02)	3.17981(-01)	2.19212(+02)	8.23205(-03)	5.19877(-05)	3.96606(+01)	2.64155(+00)
320	2.90442(-05)	3.84679(-05)	2.90442(-05)	1.34220(-03)	1.99991(-06)	3.28414(-06)	8.10996(-06)
640	2.01537(-11)	2.01373(-11)	2.01537(-11)	4.49640(-15)	4.21885(-15)	4.10783(-15)	4.05231(-15)

Table 3.4: Maximum Absolute Relative Errors of Various Third Order Methods with respect to the Number of Steps $(y_2(x))$ *(Problem 3.3)*

N	**Lambert & Shaw (1965)**	**Van Niekerk (1987)**	**Van Niekerk (1988)**	**Ikhile (2001)**	**3-ERM(1)**	**3-ERM(2)**	**3-MERM**
160	2.18514(-01)	5.06153(-04)	2.18514(-01)	5.28030(-03)	3.14264(-05)	4.72343(-02)	2.00709(-04)
320	2.16581(-06)	2.16300(-06)	2.16581(-06)	7.00650(-05)	1.86383(-07)	6.49753(-07)	6.70213(-07)
640	1.96714(-11)	1.96536(-11)	1.96714(-11)	4.10783(-15)	2.77556(-15)	2.33147(-15)	2.88658(-15)

Table 3.5: Maximum Absolute Relative Errors of Various Third Order Methods with respect to the Number of Steps (Problem 3.4)

N	**Lambert & Shaw (1965)**	**Van Niekerk (1987)**	**Van Niekerk (1988)**	**Ikhile (2001)**	**3-ERM(1)**	**3-ERM(2)**	**3-MERM**
1280	2.91323(-05)	1.67276(-04)	2.91323(-05)	2.15408(-05)	7.46251(-04)	1.68219(-04)	3.74217(-05)
2560	3.12721(-06)	1.56050(-05)	3.12721(-06)	3.18139(-06)	3.31054(-06)	2.48349(-05)	4.58719(-06)
5120	3.67925(-07)	1.24983(-06)	3.67925(-07)	4.38761(-07)	1.96674(-07)	1.16168(-06)	5.65849(-07)

Table 3.6: Maximum Absolute Relative Errors of Various Third Order Methods with respect to the Number of Steps (Problem 3.5)

N	**Lambert & Shaw (1965)**	**Van Niekerk (1987)**	**Van Niekerk (1988)**	**Ikhile (2001)**	**3-ERM(1)**	**3-ERM(2)**	**3-MERM**
16	2.39514(-02)	2.10235(-01)	2.39514(-02)	5.20857(-04)	3.93191(+00)	1.51616(-01)	4.46280(-01)
32	5.73126(-03)	5.01590(-02)	5.73126(-03)	6.22138(-05)	5.87270(+00)	3.47699(-02)	9.22318(-02)
64	1.72803(-02)	2.15491(-01)	1.72803(-02)	9.67085(-05)	4.01475(+00)	1.52879(-01)	3.74109(-01)

3.8 Discussions and Conclusions

From Table 3.1, we can see that the third order rational method of Ikhile (2001) and Van Niekerk (1987) generated the least accurate numerical results, while the remaining third order rational methods by Lambert & Shaw (1965) and Van Niekerk (1988) are found to have comparable accuracy in solving *Problem 3.1*. Our new 3-MERM turned out to have better accuracy compared to other existing third order rational methods. The third order methods 3-ERM(1) and 3-ERM(2) are unable to return any result because this problem causes the expressions c_2 in (3.28) and (3.29) to become undefined.

Problem 3.2 is indeed a very stiff, non-autonomous problem. From Table 3.2, we can see that 3-MERM and 3-ERM(1) generated results that are comparable in accuracy for $N = 10000$ and $N = 100000$ in solving *Problem 3.2*, followed by 3-ERM(2). Third order rational methods by Lambert & Shaw (1965), Van Niekerk (1987), Van Niekerk (1988) and Ikhile (2001) are found to have comparable accuracy for $N = 1000$, 10000 and 100000, except for Ikhile (2001) which converged slowly to the exact solution for $N = 100000$.

Problem 3.3 is a stiff system, but less 'stiffer' than *Problem 3.2*. From Table 3.3 and Table 3.4, we can see that 3-ERM(1) generated satisfying results for $N = 160$ compared to other third order rational methods. In view of this, we can say that 3-ERM(1) is potential to achieve high accuracy with a smaller number of integration steps. 3-MERM and 3-ERM(2) are only found to have comparable accuracy for $N = 320$ and $N = 640$. Numerical results generated by the third order rational methods of Lambert & Shaw (1965), Van Niekerk (1987) and Van Niekerk (1988) are less satisfying for $N = 160$ especially when computing the component $y_1(x)$.

Problem 3.4 is a stiff system arises from the reduction of a second order initial value problem to a system of coupled first order differential equations. From Table 3.5, it can be seen that 3-MERM, 3-ERM(1), third order rational methods of Lambert & Shaw (1965), Van Niekerk (1988) and Ikhile (2001) are found to have comparable accuracy except for $N = 1280$. On the other hand, 3-ERM(2) and third order method of Van Niekerk (1987) are found to have comparable accuracy in solving *Problem 3.4* for any number of integration steps.

Lastly, the results from Table 3.6 clearly showed that the third order rational method of Ikhile (2001) is the most suitable method in solving a problem whose solution possesses singularity because it yields more accurate numerical results. 3-MERM, 3-ERM(2) and the third order rational method of Van Niekerk (1987) are comparable in accuracy; while the third order rational methods of Lambert & Shaw (1965) and Van Niekerk (1988) are comparable. 3-ERM(1) returns the least satisfying results among all third order rational methods.

CHAPTER FOUR

VARIABLE STEP-SIZE STRATEGY FOR

ONE-STEP RATIONAL METHODS

4.1 Introduction

An efficient integrator must be able to change the step-size because it is needed to ensure that the step-size is small enough to generate numerical results up to certain accuracy, and at the same time, to ensure the step-size is large enough to avoid unnecessary computational work (Hairer *et al.*, 1993; Butcher, 2008). In this chapter, a variable step-size strategy adopted from Butcher (2008) and is introduced to be applied to one-step rational methods. We also showed that the adopted variable step-size strategy which is originally for Runge-Kutta methods could be easily extended to other one-step numerical schemes such as one-step rational methods.

4.2 The Variable Step-size Strategy

Consider the numerical integration of the initial value problem

$$y'(x) = f\left(x, y(x)\right),\ y(a) = \eta,\ f : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m,\ x \in [a,b],$$

for the following discussions of variable step-size strategy. Before the numerical integration started, an initial step-size, say h_0 is selected. The programme then computes two approximations to the solution, y_1 and $\hat{y}_1$. First, the value y_1 is obtained with step-size h_0. After that, integrate twice along the same interval $[a,b]$ by halving the step-size h_0 i.e. $h_0/2$, yields the value of $\hat{y}_1$. Then an estimate of the error for the less precise result is $\|\hat{y}_1 - y_1\|$. We want this error estimation to satisfy

$$\|\hat{y}_1 - y_1\|_\infty \le Tol, \tag{4.1}$$

where *Tol* is the desired tolerance prescribed by the user. If the inequality (4.1) is satisfied, then the computed step is accepted and this also means that y_1 is accepted and will be used to compute y_2 with the same step-size h_0. However, if

$$\left\|\hat{y}_1 - y_1\right\|_\infty > Tol \tag{4.2}$$

is satisfied, then the computed value of y_1 and step-size h_0 are rejected. Following this, y_1 has to be recalculated using a new step-size, say h_1. The new step-size h_1 is obtained using the formulae:

$$h_1 = h_0 \times r \,, \tag{4.3}$$

where

$$r = \min\left(\max\left(0.5, 0.9\left(\frac{Tol}{\left\|\hat{y}_1 - y_1\right\|_\infty} \right)^{\frac{1}{p+1}} \right), 2.0 \right). \tag{4.4}$$

From equation (4.4), we note that *p* is the order of the rational method, and *Tol* is the same user prescribed tolerance shown in (4.1) and (4.2). Equation (4.3) showed that the new step-size h_1 is in fact the step-size h_0 being adjusted by the factor *r* from equation (4.4).

After obtaining h_1, the programme then computes two new solutions, say $y_{1(new)}$ and $\hat{y}_{1(new)}$. As mentioned earlier, the value $y_{1(new)}$ is obtained with step-size h_1. After that, integrate twice along the same interval $\left[a,b\right]$ by halving the step-size h_1 i.e. $h_1/2$, yields the value of $\hat{y}_{1(new)}$. Then, the validation processes take place using the inequalities

$$\left\|\hat{y}_{1(new)} - y_{1(new)}\right\|_\infty \le Tol \,, \tag{4.5}$$

or

$$\left\|\hat{y}_{1(new)} - y_{1(new)}\right\|_{\infty} > Tol\ . \tag{4.6}$$

If (4.5) is satisfied, then the step-size h_1 is accepted. This also means that $y_{1(new)}$ is accepted and will be used to compute y_2 with the same step-size h_1. If (4.6) is satisfied, the step-size h_1 and the current solution $y_{1(new)}$ are rejected and a new adjusted step-size, say h_2 will be identified using equations

$$h_2 = h_1 \times r\ , \tag{4.7}$$

where

$$r = \min\left(\max\left(0.5, 0.9\left(\frac{Tol}{\left\|\hat{y}_{1(new)} - y_{1(new)}\right\|_{\infty}}\right)^{\frac{1}{p+1}}\right), 2.0\right). \tag{4.8}$$

Finally, the process to recalculate a new y_1 is carried out again using the new adjusted step-size h_2 until the error estimation is less than the prescribed tolerance.

As the computation progresses, the error estimations in (4.1) and (4.5) can be generalized to

$$\left\|\hat{y}_i - y_i\right\|_{\infty} \le Tol\ , \tag{4.9}$$

where $i \ge 1$ are some positive integers. Similar generalization for (4.2) and (4.6) is given by

$$\left\|\hat{y}_i - y_i\right\|_{\infty} > Tol\ . \tag{4.10}$$

Formulae for the new step-size stated in equations (4.3) and (4.7) and their corresponding r in equations (4.4) and (4.8) can be generalized as

$$h_{n+1} = h_n \times r\ ,\ n = 0,1,2,3,\ldots, \tag{4.11}$$

and

$$r = \min\left(\max\left(0.5, 0.9\left(\frac{Tol}{err}\right)^{\frac{1}{p+1}} \right), 2.0 \right), \tag{4.12}$$

respectively. We note that *err* is the generalized error estimation $\|\hat{y}_i - y_i\|_\infty$, *Tol* is the user prescribed tolerance, and *p* is the order of the underlying rational method. Let's briefly explain equation (4.12). From equation (4.12), $(Tol/err)^{\frac{1}{p+1}}$ 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 h_{n+1} is also accepted (Butcher, 2008; Hairer *et al*., 1993). Furthermore, to prevent the step-size h_{n+1} from increasing or decreasing too fast, the step-size ratio was usually forced to lie between two bounds such as 0.5 and 2.0 (Hairer *et al.*, 1993; Butcher, 2008).

While applying 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_n is accepted at the point x_i, we must check whether the next point, say x_{i+1} (or equivalent to $x_i + h_n$) still lie in the interval $[a,b]$ i.e.

$$x_{i+1} < b. \tag{4.13}$$

If (4.13) is satisfied, then the computation continues without any interruption. However, if x_{i+1} is found to coincide with or greater than the right boundary *b* i.e.

$$x_{i+1} \geq b, \tag{4.14}$$

then the programme immediately rejects x_{i+1} and the current step-size h_n . The current step-size h_n is then replaced by a final step-size, say h_b which can be obtained using the formula

$$h_b = b - x_i \,. \tag{4.15}$$

Lastly, the programme will perform a last integration to obtain the numerical approximation at the point $x = b$, say y_b, using the new step-size h_b obtained from (4.15).

Similar routine is applied when a step-size h_n is rejected at the point x_i. When a step-size h_n is rejected, the current x_i and y_i are also rejected. A new x_i is then recalculated using the new step-size h_{n+1}. This time, we want to check whether the new x_i (or equivalent to $x_{i-1} + h_{n+1}$) still lie in the interval $[a,b]$ i.e.

$$x_i < b \,. \tag{4.16}$$

If (4.16) is satisfied, then the programme continues finding the new y_i using the new step-size h_{n+1}. On the contrary, if the new x_i is found to coincide with or greater than the right boundary *b* i.e.

$$x_i \ge b \,, \tag{4.17}$$

then the programme immediately rejects x_i and the step-size h_{n+1}. The step-size h_{n+1} is then replaced by a final step-size, say h_b which can be computed using the formula

$$h_b = b - x_{i-1} \,. \tag{4.18}$$

Lastly, the programme will perform a last integration to obtain the numerical approximation at the point $x = b$, say y_b, using the new step-size h_b obtained from

(4.18). Finally, we summarized the flow of the variable step-size strategy presented in this section in Figure 4.1, Figure 4.2 and Figure 4.3.

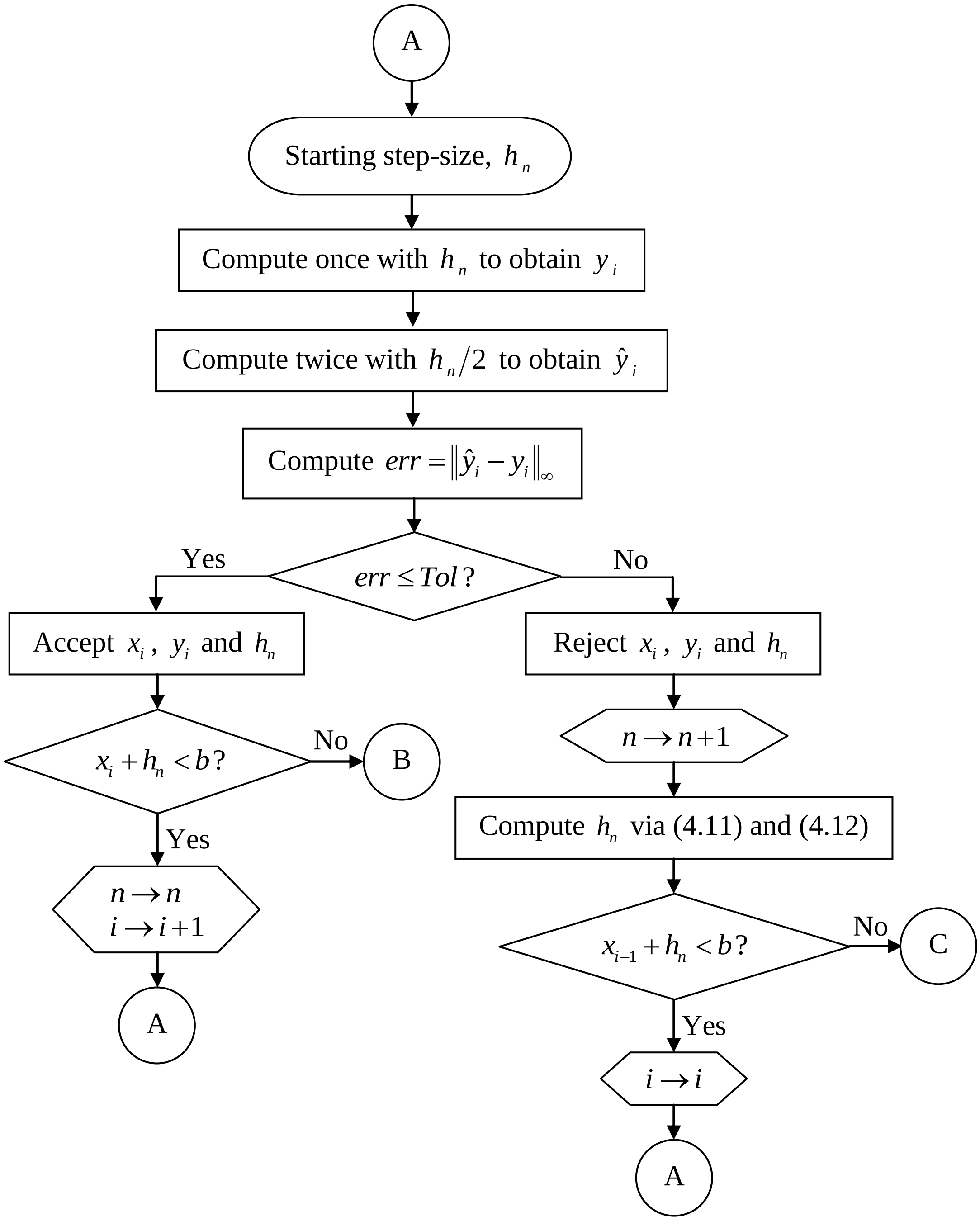

Figure 4.1 Main routine (A)

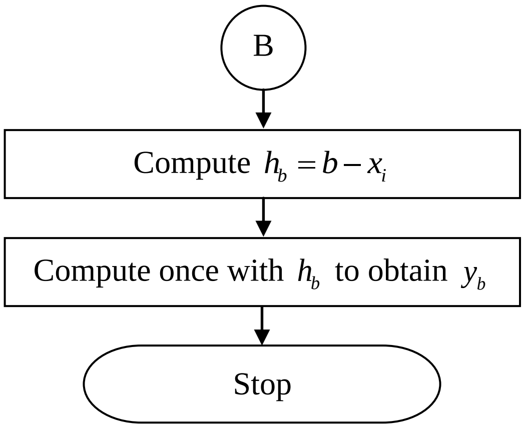

Figure 4.2 Subroutine (B) to compute y_b

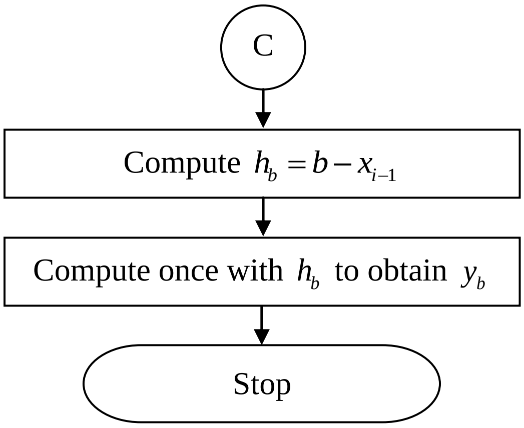

Figure 4.3: Subroutine (C) to compute y_b

4.3 Numerical Experiments and Comparisons

In this section, we solved *Problem 4.1 – Problem 4.5* with the variable step-size strategy described in this Section 4.2, using the third order MERM (as in (3.23)) and existing third order rational methods from Lambert & Shaw (1965) (as in (3.24)), Van Niekerk (1987) (as in (3.25)), Van Niekerk (1988) (as in (3.26)), Ikhile (2001) (as in (3.27)) and Teh & Yaacob (2013b) (as in (3.28) and (3.29)). For the case of constant step-size, it is sufficient to present the maximum absolute relative errors over the interval of integration $[a,b]$ as described in Section 3.7.

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 method used in comparison,

c. STEP as the total number of successful steps within the interval $[a,b]$, and

d. MAXE as the maximum absolute relative error defined by $\max_{0\le n\le \mathrm{STEP}}\{|y(x_n)-y_n|\}$.

We note that $y(x_n)$ and y_n represents the theoretical solution and numerical solution of a test problem at point x_n. We also note that $q=3$ for *Problem 4.1 – Problem 4.5*.

Problem 4.1

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

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

Problem 4.2 (Fatunla, 1982)

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

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

Problem 4.3 (Ramos, 2007)

$$y_1'(x)=-1002y_1(x)+1000y_2(x)^2,\ y_1(0)=1,\ x\in[0,1];$$

$$y_2'(x)=y_1(x)-y_2(x)\big(1+y_2(x)\big),\ y_2(0)=1,\ x\in[0,1];$$

The theoretical solutions are $y_1(x)=e^{-2x}$ and $y_2(x)=e^{-x}$.

Problem 4.4 (Yaakub and Evans, 2003)

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

The theoretical solution is $y(x)=0.01e^{-100x}+e^{-x}$. *Problem 4.4* 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 $y_2(x)=-e^{-100x}-e^{-x}$.

Problem 4.5 (Ramos, 2007)

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

The theoretical solution is $y(x)=\tan(x+\pi/4)$. From the theoretical solution, notice that the solution becomes unbounded in the neighbourhood of the singularity at $x=\pi/4\approx 0.785398163367448$.

Table 4.1: Comparisons of Various Third Order Rational Methods in Solving Problem 4.1 $(h_0 = 0.1)$

TOL	METHOD	STEP	MAXE
	Lambert & Shaw (1965)	5	1.72972(-04)
	Van Niekerk (1987)	5	4.88854(-03)
	Van Niekerk (1988)	5	1.72972(-04)
10^{-2}	Ikhile (2001)	5	1.43693(-03)
	3-ERM(1)	-	-
	3-ERM(2)	-	-
	3-MERM	5	1.40311(-05)
	Lambert & Shaw (1965)	6	1.10009(-04)
	Van Niekerk (1987)	49	1.16717(-04)
	Van Niekerk (1988)	6	1.10009(-04)
10^{-4}	Ikhile (2001)	13	1.15537(-04)
	3-ERM(1)	-	-
	3-ERM(2)	-	-
	3-MERM	5	1.40311(-05)
	Lambert & Shaw (1965)	33	1.13273(-06)
	Van Niekerk (1987)	332	1.14899(-06)
	Van Niekerk (1988)	33	1.13273(-06)
10^{-6}	Ikhile (2001)	64	1.14626(-06)
	3-ERM(1)	-	-
	3-ERM(2)	-	-
	3-MERM	12	1.27510(-06)

Table 4.2: Comparisons of Various Third Order Rational Methods in Solving Problem 4.2 $(h_0 = 0.0001)$

TOL	METHOD	STEP	MAXE
10^{-2}	Lambert & Shaw (1965)	10001	1.10728(-06)
	Van Niekerk (1987)	10001	1.89317(-06)
	Van Niekerk (1988)	10001	1.10728(-06)
	Ikhile (2001)	10001	1.44295(-05)
	3-ERM(1)	10001	2.86596(-08)
	3-ERM(2)	10001	6.42108(-07)
	3-MERM	10001	3.33495(-08)
10^{-4}	Lambert & Shaw (1965)	10001	1.10728(-06)
	Van Niekerk (1987)	10001	1.89317(-06)
	Van Niekerk (1988)	10001	1.10728(-06)
	Ikhile (2001)	10001	1.44295(-05)
	3-ERM(1)	10001	2.86596(-08)
	3-ERM(2)	10001	6.42108(-07)
	3-MERM	10001	3.33495(-08)
10^{-6}	Lambert & Shaw (1965)	10001	1.10728(-06)
	Van Niekerk (1987)	-	-
	Van Niekerk (1988)	10001	1.10728(-06)
	Ikhile (2001)	-	-
	3-ERM(1)	10001	2.86596(-08)
	3-ERM(2)	10001	6.42108(-07)
	3-MERM	10001	3.33495(-08)

Table 4.3: Comparisons of Various Third Order Rational Methods in Solving Problem 4.3 $(y_1(x))$ $(h_0 = 0.1)$

TOL	METHOD	STEP	MAXE
10^{-2}	Lambert & Shaw (1965)	167	1.06219(-02)
	Van Niekerk (1987)	165	1.03222(-02)
	Van Niekerk (1988)	167	1.06219(-02)
	Ikhile (2001)	141	1.60290(-02)
	3-ERM(1)	10	7.82458(-03)
	3-ERM(2)	156	1.36322(-02)
	3-MERM	148	1.04070(-02)
10^{-4}	Lambert & Shaw (1965)	191	1.09986(-04)
	Van Niekerk (1987)	189	1.12825(-04)
	Van Niekerk (1988)	191	1.09986(-04)
	Ikhile (2001)	395	8.97524(-05)
	3-ERM(1)	93	1.56436(-04)
	3-ERM(2)	160	1.22566(-04)
	3-MERM	162	1.14548(-04)
10^{-6}	Lambert & Shaw (1965)	476	7.92328(-07)
	Van Niekerk (1987)	477	8.10994(-07)
	Van Niekerk (1988)	476	7.92328(-07)
	Ikhile (2001)	385	7.17341(-07)
	3-ERM(1)	397	7.32652(-07)
	3-ERM(2)	441	1.01760(-08)
	3-MERM	1005	8.79066(-07)

Table 4.4: Comparisons of Various Third Order Rational Methods in Solving Problem 4.3 $\left(y_2\left(x\right)\right)$ $\left(h_0 = 0.1\right)$

TOL	METHOD	STEP	MAXE
10^{-2}	Lambert & Shaw (1965)	167	1.33297(-04)
	Van Niekerk (1987)	165	1.34738(-04)
	Van Niekerk (1988)	167	1.33297(-04)
	Ikhile (2001)	141	6.08929(-03)
	3-ERM(1)	10	2.89992(-03)
	3-ERM(2)	156	1.72521(-04)
	3-MERM	148	5.32186(-05)
10^{-4}	Lambert & Shaw (1965)	191	3.65677(-05)
	Van Niekerk (1987)	189	3.68719(-05)
	Van Niekerk (1988)	191	3.65677(-05)
	Ikhile (2001)	395	9.53541(-08)
	3-ERM(1)	93	9.90454(-05)
	3-ERM(2)	160	1.78079(-05)
	3-MERM	162	1.25284(-05)
10^{-6}	Lambert & Shaw (1965)	476	3.63422(-09)
	Van Niekerk (1987)	477	3.72452(-09)
	Van Niekerk (1988)	476	3.63422(-09)
	Ikhile (2001)	385	1.14095(-09)
	3-ERM(1)	397	1.22592(-09)
	3-ERM(2)	441	1.02564(-11)
	3-MERM	1005	2.05168(-09)

Table 4.5: Comparisons of Various Third Order Rational Methods in Solving Problem 4.4 $(h_0 = 0.1)$

TOL	METHOD	STEP	MAXE
	Lambert & Shaw (1965)	958	7.88256(-05)
	Van Niekerk (1987)	1611	7.79836(-05)
	Van Niekerk (1988)	958	7.88256(-05)
10^{-2}	Ikhile (2001)	521	3.66823(-04)
	3-ERM(1)	399	9.84281(-04)
	3-ERM(2)	1593	8.78372(-05)
	3-MERM	694	2.33427(-04)
	Lambert & Shaw (1965)	4334	1.03121(-06)
	Van Niekerk (1987)	10667	1.06762(-07)
	Van Niekerk (1988)	4334	1.03121(-06)
10^{-4}	Ikhile (2001)	1893	7.35386(-06)
	3-ERM(1)	1227	1.15590(-04)
	3-ERM(2)	7927	3.07927(-07)
	3-MERM	3357	3.15480(-06)
	Lambert & Shaw (1965)	21856	1.07760(-08)
	Van Niekerk (1987)	80389	5.74256(-09)
	Van Niekerk (1988)	21856	1.07760(-08)
10^{-6}	Ikhile (2001)	9781	1.13378(-07)
	3-ERM(1)	123196	1.16102(-06)
	3-ERM(2)	56182	6.46744(-09)
	3-MERM	17083	3.41138(-08)

Table 4.6: Comparisons of Various Third Order Rational Methods in Solving Problem 4.5

TOL	h_0	**METHOD**	**STEP**	**MAXE**
		Lambert & Shaw (1965)	-	-
		Van Niekerk (1987)	-	-
		Van Niekerk (1988)	-	-
	0.1	Ikhile (2001)	8	8.31976(-03)
		3-ERM(1)	-	-
		3-ERM(2)	-	-
		3-MERM	-	-
		Lambert & Shaw (1965)	80	1.84024(-03)
		Van Niekerk (1987)	-	-
		Van Niekerk (1988)	80	1.84024(-03)
10^{-2}	0.01	Ikhile (2001)	80	8.28983(-06)
		3-ERM(1)	-	-
		3-ERM(2)	-	-
		3-MERM	-	-
		Lambert & Shaw (1965)	800	2.43201(-04)
		Van Niekerk (1987)	800	4.43592(-03)
		Van Niekerk (1988)	800	2.43201(-04)
	0.001	Ikhile (2001)	800	1.16650(-07)
		3-ERM(1)	-	-
		3-ERM(2)	800	3.08424(-03)
		3-MERM	800	6.31692(-03)

4.4 Discussions and Conclusions

From Table 4.1, all third order rational methods require 5 successful steps within the interval $\left[0, 0.5\right]$ when the prescribed tolerance is 10^{-2}. However, 3-MERM turned out to have better accuracy compared to other existing third order rational methods in solving *Problem 4.1*. 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 (1987) and a slight increase in the number of successful steps for the third order method of Ikhile (2001). On the other hand, the number of successful steps for the methods of Lambert & Shaw (1965), Van Niekerk (1988) and 3-MERM remain (or almost) unchanged. In the case when the prescribed tolerance is 10^{-4}, 3-MERM 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 $\left[0, 0.5\right]$. We can see that 3-MERM is the cheapest in computational cost, followed by Lambert & Shaw (1965), Van Niekerk (1988), Ikhile (2001), and lastly Van Niekerk (1987). For all three case, the third order methods 3-ERM(1) and 3-ERM(2) are unable to return any result because this problem causes the expressions c_2 in (3.28) and (3.29) became undefined. However, it doesn't mean that 3-ERM(1) and 3-ERM(2) failed to solve non-autonomous problem such as *Problem 4.1*.

Problem 4.2 is indeed a very stiff differential problem, as the initial step-size 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 4.2 that, all third order rational methods required 10001 successful steps within the interval $[0,1]$ for all three prescribed tolerance 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. As the total number of successful steps are the same, we can see that 3-ERM(1) and 3-MERM generated results that are comparable in accuracy and also more accurate compared to other existing third order rational methods. We wish to point out that: third order method of Van Niekerk (1987) failed to converge while third order method of Ikhile (2001) suffered too many step-size rejections when the accepted error estimate is set to be bounded by 10^{-6}. Therefore, there are a few things that need to be considered when solving non-autonomous 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.

Problem 4.3 is also a stiff problem but less 'stiffer' than *Problem 4.2*. From Table 4.3 and when the tolerance is 10^{-2}, we have observed that 3-ERM(1) required only 10 successful steps to achieve better accuracy compared to other existing methods in computing the component $y_1(x)$. However, this is not the case when computing the component $y_2(x)$ because 3-MERM turned out to be the most accurate method with 148 successful steps and almost comparable to the rest of the methods, as shown in Table 4.4. When the tolerance is decreased to 10^{-4}, the numerical results for both components $y_1(x)$ and $y_2(x)$ all seem to follow a similar pattern previously observed in the case of 10^{-2}. Third order method of Ikhile (2001) achieved better accuracy compared to other methods but with 395 successful steps, that are almost twice the number of successful steps of Lambert & Shaw (1965) and Van Niekerk

(1988). However, the increase in the number of successful steps also improve the accuracy and this is obviously seen in Table 4.4, where third order method of Ikhile (2001) achieved far more accurate result compared to other third order rational methods in computing the component $y_2(x)$. Finally, when the prescribed tolerance is set to 10^{-6}, we note that 3-ERM(2) turned out to have the best accuracy in computing both components $y_1(x)$ and $y_2(x)$. Except for 3-MERM which suffered from a certain amount of step-size rejection, remaining rational methods demonstrated almost comparable number of successful steps. The initial step-size $h_0 = 0.1$ does not cause any difficulty to obtain the approximated solution for this stiff problem.

Problem 4.4 is a stiff system arises from the reduction of a second order initial value problem to a system of coupled first order differential equations. From Table 4.5, when the prescribed tolerance is 10^{-2}, 3-ERM(1) is the cheapest method if an accuracy of 10^{-4} is desired. Alternatively, one can choose the third order methods of Lambert & Shaw (1965) or Van Niekerk (1988) if an accuracy of 10^{-5} is preferable with 958 successful steps. When the tolerance is decreased to 10^{-4}, 3-ERM(1) still remain as the cheapest method but its maximum absolute relative error is unsatisfactory compared to other third order methods. We would recommend the third order method of Ikhile (2001) due to its maximum absolute relative error and also the total number of successful steps. Third order method of Van Niekerk (1987) and 3-ERM(2) are not recommended due to their 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 third order method of Ikhile (2001) could be a good choice. If we wish to have a balance between computational cost and accuracy, we would recommend 3-MERM or perhaps even the third order methods of Lambert & Shaw (1965) and Van Niekerk (1988). If our only concern is the accuracy, then 3-ERM(2) could be the first choice followed by Van Niekerk (1987). We note that 3-ERM(1) is quite unsatisfactory in terms of computational cost and accuracy. The initial step-size $h_0 = 0.1$ works just fine for this stiff system.

We would like to discuss *Problem 4.5* and Table 4.6 in a different manner as the presentation of Table 4.6 is also different from the previously shown tables. *Problem 4.5* is a problem whose solution possesses singularity at $x = \pi/4 \approx 0.785398163367448$. Since we are using variable step-size, either one of the following situations could happen: the computed step-size h_n could overstep the singularity or it couldn't; both somehow affected by the prescribed tolerance. We shall not face this kind of difficulty if constant step-size strategy is implemented. As we can observe from Table 4.6, the prescribed tolerance is set to 10^{-2} with three different initial step-size $h_0 = 0.1$, 0.01 and 0.001. We have found out that using stricter prescribed tolerance such as 10^{-4} or 10^{-6} will generate step-size h_n that could not overstep the singularity and hence causing divergence in the approximated solution. When the initial step-size is $h_0 = 0.1$, we can see that only the third order rational method of Ikhile (2001) is able to return converging numerical solution with only 8 successful steps. When the initial step-size is decreased to $h_0 = 0.01$, more methods are returning converging solution, but the method of Ikhile (2001) generated results of better accuracy. Finally, when the initial step-size is further decreased to

$h_0 = 0.001$, third order methods of Ikhile (2001) still outperformed other third order rational methods. After several tests, we note that 3-ERM(1) failed to generate any converging numerical solution even with the initial step-size $h_0 = 0.0001$ and $h_0 = 0.00001$, using the same tolerance 10^{-2}. The interval of integration for this problem is $[0, 0.8]$. It has been shown in Table 4.6 that, initial step-size $h_0 = 0.1$, 0.01 and 0.001 required a total of 8, 80 and 800 successful steps respectively, to return converging numerical solution. In other words, there is no step-size rejection occurred during the integration along the interval $[0, 0.8]$, using these three initial step-size.

CHAPTER FIVE

SUMMARY AND CONCLUSION

The ideas of the research work contained in this report are twofold: (i) the discoveries of a new class of explicit one-step modified exponential-rational methods, and (ii) the proposal of a variable step-size strategy and implementation to several one-step rational methods.

After a short introduction in Chapter 1 and some literature review to support the rationale of our studies in Chapter 2, the main contributions of this research begin with Chapter 3. In Chapter 3, we have presented a new class of modified exponential-rational methods (MERMs) which are explicit one-step methods that are based on rational functions. The general formulation of MERM is given in (3.2) while the order condition and local truncation error for a MERM are explained in Definition 3.1 and Definition 3.2. The parameters b, c and a_j for $j = 0,1,\ldots,k$ are generalized in Section 3.3 and the generalized formulae were shown in equations (3.8) – (3.11). On choosing an integer of $p \geq 2$ (i.e. the order of a MERM), the parameters for a specific MERM can be determined and these parameters are unique for a chosen integer. The principal local truncation error term is also generalized as in equation (3.13). Sections 3.5 and 3.6 showed that each MERM is L-stable, consistent by Definition 3.3 and convergence for any order or accuracy. We have chosen some test problems to evaluate the effectiveness of MERMs and other existing rational methods in terms of numerical accuracy. From the numerical experiments conducted, MERMs and ERMs from Teh & Yaacob (2013b) are found to have comparable accuracy, and they generated more accurate numerical results compared to existing rational methods of Lambert & Shaw (1965), Van Niekerk (1987), Van Niekerk (1988) and Ikhile (2001) in solving non-stiff problem (*Problem 3.1*) and stiff problems (*Problems 3.2*, *3.3* and *3.4*). All these tests seem to indicate that MERMs are suitable and more reliable for general initial value problems whose solutions possess no singularities. However, MERMs are not suitable for problems whose solutions possess singularities, as was shown in Table 3.6. Finally, MERMs and ERMs of Teh & Yaacob (2013b) are comparable in terms of numerical accuracy. However, we suggest MERMs over ERMs for the numerical solution of first order initial value problem because MERMs are uniquely defined but ERMs are not uniquely defined as explained in Chapter 1 and Chapter 2.

In Chapter 4, we have discussed and presented a variable step-size strategy to be implemented together with one-step rational methods. Detailed explanation on the strategy is carried out in Section 4.2 and the strategy is further summarized in three flow charts shown in Figure 4.1, Figure 4.2 and Figure 4.3. We have chosen some test problems to evaluate the implementation of variable step-size strategy in several selected third order rational methods from the literature. The evaluation is based on the total number of successful steps needed to complete the integration along the interval $\left[a,b\right]$; and the maximum absolute relative errors correspond to the prescribed tolerance and also total number of successful steps. Numerical experimentations showed that the proposed variable step-size strategy is workable in all selected rational methods. However, there are some needs of precautions especially in solving stiff problem and problem whose solution possesses singularity. These precautions are selection of initial step-size and selection of prescribed tolerance for the error estimation. The variable step-size strategy could be improved by introducing another subroutine to control the step-size h_n so that it would overstep the singularity and convergence of numerical solution is guaranteed when solving problem whose solution possesses singularity. In our research, the initial step-size was supplied by the user to the code based on his/her mathematical knowledge or previous experience. According to Hairer *et al*. (1993), a bad choice of the initial step-size will be quickly adjusted by the step-size control but nevertheless, when this happens too often and when the initial guess of step-size is too bad, much computing time can be wasted. Therefore, future improvement of our proposed variable step-size strategy would include subroutine to let the computer decide the initial step-size. Another suggested improvement is to introduce a straightforward mechanism of doubling the step-size i.e.

$$h_{n+1} = 2h_n, \tag{5.1}$$

if specified error estimation is fulfilled. For example, Butcher (2008) suggested the adjusted step-size in equation (5.1) if the error estimation is less than $0.04 \times Tol$. The motive of doubling the step-size is to accelerate the numerical integration and at the same time, avoiding unnecessarily excessive small step-size which contributed to extra computational cost. All these suggestions will be considered in future study.

With the above summary and conclusion, we conclude this report.

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