ACKNOWLEDGEMENTS

I wish to express my deepest gratitude to my main supervisor, Assoc. Prof. Dr. Nazeeruddin Yaacob and co-supervisor, Dr. Norma Alias; who have suggested the research topic and directed the research. I thank them for their enduring patience, contributing ideas, discussing plans, and encouraging support during the course of my study.

I further wish to express my gratitude to the Universiti Teknologi Malaysia for providing a variety of helpful facilities in order for me to complete my study conveniently.

Finally, I would like to dedicate this text to my parents and my wife for their endless love, care and financial support.

ABSTRACT

Unconventional methods for the numerical solution of first order initial value problems (IVPs) are well established in the past decades. There are two major reasons that motivate the developments of unconventional methods: firstly, unconventional methods are developed to solve certain types of IVPs, such as IVPs with oscillatory solutions or IVPs whose solutions possess singularities, where in most of the time, conventional methods will perform poorly; and secondly, unconventional methods might possess some outstanding features that could never be achieved by conventional methods. These features include achieving high order of numerical accuracy with less computational cost, stronger stability properties and so on. In this thesis, some studies are made of the unconventional methods based on rational functions and mean expressions. The study has led to the discovery of some new exponential-rational methods and rational multistep methods which can be used effectively for numerical solution of first order IVPs. The study continues with the discoveries of some new pseudo Runge-Kutta methods based on harmonic and arithmetic means; and a multistep method based on centroidal mean, which are found to be effective for the numerical solution of first order IVPs. This thesis also includes the study of implicit Runge-Kutta (IRK) methods, which led to the developments of three new classes of IRK methods based on Kronrod-type quadrature formulae. Each new method developed in this thesis is furnished with local truncation error and absolute stability analysis. In addition, each new method is tested on some test problems and also compared with other conventional or classical methods in the same order.

ABSTRAK

Kaedah-kaedah tak konvensional untuk penyelesaian masalah-masalah nilai awal (MNA) peringkat pertama secara berangka sudah wujud beberapa dekad yang lalu. Terdapat dua sebab utama yang memotivasikan pembangunan kaedah-kaedah tak konvensional: pertamanya, kaedah-kaedah tak konvensional dibangunkan untuk menyelesaikan MNA yang tertentu seperti MNA yang mempunyai penyelesaian yang berayun atau MNA yang mempunyai penyelesaian singular, sedangkan kaedah-kaedah konvensional tidak dapat diaplikasikan dengan baik; dan keduanya, kaedah-kaedah tak konvensional mungkin memiliki beberapa sifat yang unggul yang tidak dapat dimiliki oleh kaedah-kaedah konvensional. Sifat-sifat ini termasuk pencapaian ketepatan berangka yang tinggi dengan kos pengiraan yang rendah, kestabilan yang lebih baik dan sebagainya. Dalam tesis ini, beberapa kajian telah dilakukan ke atas kaedah-kaedah tak konvensional yang berasaskan fungsi-fungsi nisbah dan ungkapan-ungkapan min. Kajian tersebut telah membawa kepada penemuan beberapa kaedah eksponen-nisbah dan kaedah multilangkah nisbah yang baru, yang dapat digunakan secara berkesan untuk penyelesaian MNA peringkat pertama secara berangka. Kajian diteruskan dengan penemuan beberapa kaedah Runge-Kutta jenis "pseudo" yang berasaskan min harmonik dan min aritmetik; dan suatu kaedah multilangkah yang berasaskan min sentroidal, yang didapati berkesan untuk penyelesaian MNA peringkat pertama secara berangka. Tesis ini juga mengandungi kajian tentang kaedah Runge-Kutta tersirat (RKT), lalu membawa kepada pembangunan tiga kelas kaedah RKT yang berasaskan kuadratur jenis Kronrod. Setiap kaedah baru yang dibangunkan dalam tesis ini dilengkapi dengan ralat pangkasan setempat dan analisis kestabilan mutlak. Selain itu, setiap kaedah baru telah diuji melalui beberapa masalah ujian dan juga dibandingkan dengan kaedah-kaedah konvensional atau klasik dalam peringkat yang setara.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF SYMBOLS

det	-	Determinant of a matrix
e	-	Vector of ones
h	-	Step-size
L_1	-	Norm 1
lim	-	Limits
P_j	-	Class of polynomials of degree j
Re	-	Real part of a complex number
$\mathbb{R}^m$	-	Real m element vectors
$R(z)$	-	Stability function of a one-step method
T_{n+1}	-	Local truncation error at x_{n+1}
TOL	-	Adopted error tolerance
z	-	Complex number
$\Vert\ \Vert_\infty$	-	Infinity norm
$\Vert\ \Vert$	-	Norm

LIST OF ABBREVIATIONS

ERM	-	Exponential-rational method
ERMs	-	Exponential-rational methods
GKLM-III	-	Gauss-Kronrod-Lobatto III method
GKLM-IIIA	-	Gauss-Kronrod-Lobatto IIIA method
GKLM-IIIB	-	Gauss-Kronrod-Lobatto IIIB method
GKLM-IIIC	-	Gauss-Kronrod-Lobatto IIIC method
GKLM(7,10)-III	-	7-stage tenth order Gauss-Kronrod-Lobatto III method
GKLM(7,10)-IIIA	-	7-stage tenth order Gauss-Kronrod-Lobatto IIIA method
GKLM(7,10)-IIIB	-	7-stage tenth order Gauss-Kronrod-Lobatto IIIB method
GKLM(7,10)-IIIC	-	7-stage tenth order Gauss-Kronrod-Lobatto IIIC method
GKM1	-	Gauss-Kronrod method 1
GKM1(5,8)	-	5-stage eighth order Gauss-Kronrod method 1
GKM2	-	Gauss-Kronrod method 2
GKM2(5,8)	-	5-stage eighth order Gauss-Kronrod method 2
GKRM-I	-	Gauss-Kronrod-Radau I method
GKRM-IA	-	Gauss-Kronrod-Radau IA method
GKRM-II	-	Gauss-Kronrod-Radau II method

GKRM-IIA	-	Gauss-Kronrod-Radau IIA method
GKRM(4,6)-I	-	4-stage sixth order Gauss-Kronrod-Radau I method
GKRM(4,6)-IA	-	4-stage sixth order Gauss-Kronrod-Radau IA method
GKRM(4,6)-II	-	4-stage sixth order Gauss-Kronrod-Radau II method
GKRM(4,6)-IIA	-	4-stage sixth order Gauss-Kronrod-Radau IIA method
IRK	-	Implicit Runge-Kutta
LTE	-	Local truncation error
LTEs	-	Local truncation errors
p-ERM	-	*p*-th order exponential-rational method
NLMMCeM(2,4)	-	2-step fourth order implicit non-linear method based on centroidal mean
PRKAM(3,4)	-	3-stage fourth order pseudo Runge-Kutta method based on arithmetic mean
PRKHM(2,3)	-	2-stage third order pseudo Runge-Kutta method based on harmonic mean
RMM	-	Rational multistep method
RMMs	-	Rational multistep method
RMM1(2,*p*)	-	2-step *p*-th order RMM1
RMM2(2,*p*)	-	2-step *p*-th order RMM2
RMM3(2,*p*)	-	2-step *p*-th order RMM3

LIST OF APPENDICES

CHAPTER 1

INTRODUCTION

1.1 Background of the Study

The first part of this section discusses special numerical methods that are based on non-polynomial interpolants and mean expressions while the second part is about implicit Runge-Kutta methods that are based on quadrature formulae.

1.1.1 Special Numerical Methods for Initial Value Problems

Conventional numerical methods for initial value problems of the form

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

that have been widely used nowadays are those from the class of linear multistep methods and the class of linear Runge-Kutta methods. These methods can further be categorized into explicit methods or implicit methods. Besides methods from these two classes, there are other options such as the predictor-corrector methods, hybrid methods and extrapolation methods.

All of the methods mentioned above are intended for application to the general initial value problems (1.1). When the initial value problems or the solutions are known in advance to have some special properties, then we can use special numerical methods which make use of these properties. The special properties may be some analytical properties of the function $f(x,y)$ such as stiffness; or it may be the solutions of the real life problems such as problems with oscillatory solutions and problems whose solutions possess singularities (Lambert, 1973). For example, if an initial value problem whose solutions are known to be periodic, or to oscillate with a known frequency, then numerical integration formulae based on trigonometric functions are particularly appropriate (Lambert, 1973). On the other hand, if the problems whose solutions possess singularities, then numerical integration formulae based on rational functions will be much more effective. Besides trigonometric functions and rational functions, other common 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, see, for example, Shaw (1967), Lambert (1973), Lambert (1974), Fatunla (1976), Wambecq (1976), Evans and Fatunla (1977), Fatunla (1978), Lee and Preiser (1978), Fatunla (1982), Neta and Ford (1984), Fatunla (1986), Neta (1986), Van Niekerk (1987), Van Niekerk (1988), Wu (1998), Wu and Xia (2001), Ikhile (2001), Ikhile (2002), Ikhile (2004), Ramos (2007), Okosun and Ademiluyi (2007a), and Okosun and Ademiluyi (2007b).

There is another class of special numerical methods for the numerical solutions of (1.1) which include mean expressions such as geometric mean, harmonic mean, centroidal mean and so on. For theoretical aspects and various perspectives of conventional numerical methods that incorporate mean expressions, see, for example, Evans and Sanugi (1987a), Evans and Sanugi (1987b), Sanugi (1988), Evans and Sanugi (1989), Sanugi and Evans (1990), Evans and Yaacob (1995), Yaacob and Evans (1995), Sanugi and Yaacob (1995a), Sanugi and Yaacob (1995b), Yaacob and Sanugi (1995a), Yaacob and Sanugi (1995b), Yaacob (1996), Yaacob and Evans (1997), Yaacob and Phang (2001), Murugesn *et al*. (2002), Yaakub and Evans (2003), Bįldįk and İnç (2003), Ponalagusamy and Senthilkumar (2007) and Senthilkumar (2008). Special numerical methods that include mean expressions are sometimes preferable due to cheaper computational costs with comparable or even better accuracy compare with conventional numerical methods for (1.1).

1.1.2 Implicit Runge-Kutta Methods for Initial Value Problems

One-step Runge-Kutta method which is a self-starting numerical method gains tremendous popularity for the computations of numerical solutions of (1.1). In most cases, explicit Runge-Kutta method is preferable because it allows explicit stage-by-stage implementation which is very easy to program using computer. However, numerical analysts also aware that the computational costs involving function evaluations increases rapidly as higher order requirements are imposed (Hall and Watt, 1976). Another disadvantage of explicit Runge-Kutta method is that it has relatively small interval of absolute stability, which is not suitable to solve stiff initial value problems (Fatunla, 1988). In view of this, we are thus taking interest in implicit Runge-Kutta method. In an implicit Runge-Kutta method, the explicit stage-by-stage implementation scheme enjoyed by explicit Runge-Kutta method is no longer available and needs to be replaced by an iterative computation (Butcher, 2003). Other than this computational difficulty, implicit Runge-Kutta method is an appealing method where higher accuracy can be obtained with fewer function evaluations, and it has relatively bigger interval of absolute stability. For excellent surveys and various perspectives of implicit Runge-Kutta methods, see, for example, Dekker and Verwer (1984), Butcher (1987), Lambert (1991), Hairer and Wanner (1991), Butcher (1992), Hairer *et al*. (1993), Iserles (1996) and Butcher (2003).

1.2 Statement and Scope of the Study

Among special numerical methods based on non-polynomial interpolants mentioned above, we are particularly attracted to special numerical methods based on rational functions. We address this kind of methods as rational methods. Our rationale is that rational methods can solve a variety of problem including non-stiff problems, stiff problems and most importantly solving problems whose solutions possess singularities. Various formulations of rational methods can be found in the following articles or texts: Lambert, (1973), Lambert (1974), Wambecq (1976), Fatunla (1982), Fatunla (1986), Van Niekerk (1987), Van Niekerk (1988), Ikhile

(2001), Ikhile (2002), Ikhile (2004), Ramos (2007), Okosun and Ademluyi (2007a), and Okosun and Ademiluyi (2007b). However, numerical comparisons among these rational methods have not been carried out and we still do not know which formulations are outstanding and which are not. In view of this, our studies are narrowed down in exploring the possibilities of developing new explicit rational methods which perform as effectively as the existing one or even better than the existing one.

On the other hand, the findings of trapezoidal rules and explicit Runge-Kutta methods that incorporate mean expressions are also very impressive. Therefore, in this study, we would like to explore the possibilities of incorporating mean expressions into some conventional numerical methods for (1.1) other than trapezoidal rules and explicit Runge-Kutta methods. After some extensive literature reviews, we have found out that linear multistep methods and pseudo Runge-Kutta methods can be modified into special methods that incorporate mean expressions. In this thesis, we regard all special numerical methods that are based on mean expressions as non-linear methods. We shall discuss these matters in later chapters.

Besides considering rational methods and non-linear methods based on mean expressions, we are also interested in implicit Runge-Kutta methods for the numerical solutions of (1.1). According to Dekker and Verwer (1984), Butcher (1987), Lambert (1991), Hairer and Wanner (1991), Iserles (1996), Butcher (2003) and many others, there are three classes of Gauss-Legendre type implicit Runge-Kutta methods that are based on three different Gauss-Legendre type quadrature formulae, namely Gauss-Legendre methods which are based on Gauss-Legendre quadrature formulae; Radau I, Radau IA, Radau II and Radau IIA methods which are based on Gauss-Radau quadrature formulae; and Lobatto III, Lobatto IIIA, Lobatto IIIB and Lobatto IIIC methods which are based on Gauss-Lobatto quadrature formulae. At this moment, it is natural to ask whether we can devise other types of quadrature formulae in order to develop some new implicit Runge-Kutta methods that will perform equally well or even better than the Gauss-Legendre type implicit Runge-Kutta methods mentioned above. Hence, in this thesis, we shall consider three different Kronrod-type quadrature formulae in constructing three new classes of Kronrod-type implicit Runge-Kutta methods. We note that Kronrod-type quadrature formulae include: the Gauss-Kronrod quadrature formulae, the Gauss-Kronrod-Radau quadrature formulae and the Gauss-Kronrod-Lobatto quadrature formulae, which will be discussed in Chapter 2.

1.3 Objectives of the Study

From the statements and scopes made in Section 1.2, it is clear that we are studying three different kinds of numerical methods for (1.1), namely rational methods based on rational functions, non-linear methods based on mean expressions, and implicit Runge-Kutta methods that are based on quadrature formulae. Hence, the specific objectives of our study are:

a) To develop a new class of one-step rational methods based on rational function and exponential function for the numerical solutions of (1.1);
b) To develop three new classes of 2-step explicit rational methods based on the works by Lambert (1973), Van Niekerk (1988) and Ikhile (2001) for the numerical solutions of (1.1);
c) To formulate some new non-linear pseudo Runge-Kutta methods based on harmonic mean and arithmetic mean for the numerical solutions of (1.1);
d) To formulate a new non-linear multistep method based on centroidal mean for the numerical solutions of (1.1); and
e) To develop some new implicit Runge-Kutta methods based on three different Kronrod-type quadrature formulae for the numerical solutions of (1.1).

1.4 Significance of the Study

The first aim of our study is to derive a new class of one-step rational methods from the combination of rational function and exponential function. At present, this kind of rational methods have never been reported else where. Our study shows that these rational methods do provide alternatives to current one-step rational methods shown in the literature. Besides, we also show that rational methods in multistep setting are also possible. The significance of our study in this particular research topic is that, we have introduced rational methods that contain exponential functions and also modified some existing one-step rational methods to their multistep counterparts.

The second aim of our study is to introduce a new non-linear implicit multistep method and some non-linear explicit pseudo Runge-Kutta methods that are based on mean expressions for the numerical solutions of (1.1). The significance of our study in this particular research topic is that, we have further extended some mean expressions to other types of conventional numerical methods, which have never been modified into their non-linear counterparts.

Through these years, although rational methods and non-linear methods based on mean expressions are not as popular as conventional numerical methods (e.g. linear multistep methods and Runge-Kutta methods), they have proved to be reliable in solving initial value problems which arise from various fields of applications, and also being competitive with conventional numerical methods. One can evaluate the efficiency of these numerical methods by referring to articles such as Ponalagusamy and Senthilkumar (2007); Senthilkumar (2008) and many others articles mentioned in the previous paragraphs. Besides, these numerical methods may possess some desired numerical properties that cannot be achieved by conventional numerical methods. Therefore, it is worthy to develop new rational methods and new non-linear methods based on mean expressions, which will provide new insights and new ideas for future research. We also like to attract more researchers to study these particular research topics through the publications of our findings.

The third significance of our study is the discovery of some new implicit Runge-Kutta methods that are based on three different Kronrod-type quadrature formulae. This discovery has somehow shed some lights to future research where we suggest that more implicit Runge-Kutta methods based on quadrature formulae can be developed. The newly develop implicit Runge-Kutta methods will serve as counterparts of the classical Gauss-Legendre type implicit Runge-Kutta methods. All in all, our final aim is to provide different alternatives of implicit Runge-Kutta methods for the numerical solutions of (1.1).

1.5 Outline of Thesis

In Chapter 2, we review some rational methods found in the literature, together with their rational interpolants, local truncation error analyses and stability analyses. The basic concepts of non-linear methods based on mean expressions and some examples of its kind are also given. Implicit Runge-Kutta methods based on Gauss-Legendre type quadrature formulae and the concepts of Kronrod-type quadrature formulae are also discussed.

Chapter 3 is about the developments of a new class of rational methods based on rational function and exponential function. Local truncation error and absolute stability analyses are included as well. These new methods are compared with other existing rational methods in solving some test problems.

Chapter 4 is about the developments of three new classes of 2-step rational methods. Local truncation error and absolute stability analyses are included as well. These 2-step rational methods are compared with other existing rational methods in solving some test problems. Newly developed 2-step rational methods are then generalized to form r-step rational methods.

In Chapter 5, we consider the developments of two 2-stage third order pseudo Runge-Kutta methods based on harmonic mean and a 3-stage fourth order pseudo Runge-Kutta method based on arithmetic mean. Local truncation error and absolute stability analyses for these methods are included as well. These methods are compared with conventional explicit Runge-Kutta methods and pseudo Runge-Kutta methods in the same order in solving some test problems.

In Chapter 6, we present the development of a 2-step fourth order implicit non-linear method based on centroidal mean, together with its local truncation error and absolute stability analyses. As usual, this new method is compared with conventional linear multistep method in solving some test problems.

Chapter 7 is about the developments of some new implicit Runge-Kutta methods that are based on three different Kronrod-type quadrature formulae. Order condition for each new implicit Runge-Kutta method is verified. Absolute stability analysis for each method is included as well. Last but not least, all new Kronrod-type implicit Runge-Kutta methods are compared with some classical Gauss-Legendre type implicit Runge-Kutta methods in solving some test problems.

Chapter 8 contains some summaries of our findings in this thesis and several recommendations for future research.