CHAPTER – 1

INTRODUCTION

...even if quite a low accuracy is sufficient in the solution, 
the calculation must be very accurate and should certainly be 
based on one of the more accurate methods
such as the finite difference or Runge-Kutta methods

- L. Collatz

The advent of computers has tremendously revolutionized the type and variety of numerical methods over the past three decades and these methods are applied to solve mathematical problems. This thesis is concerned with the study on extended fourth order Runge-Kutta (RK) methods based on a variety of means such as arithmetic mean, centroidal mean, harmonic mean, contraharmonic mean, heronian mean, root mean square, and geometric mean, to produce approximate solutions for Initial Value Problems (IVPs) in ordinary differential equations. Many processes, in the physical and biological sciences, engineering, and other areas are modeled by IVPs, and RK methods play a vital role in solving them.

The great diversity in differential equations indicates that a variety of different methods are needed, although a frequent approach is to replace the differential equation by a difference equation. To emphasize this, David J. Evans and his team of researchers who introduced a new dimension to the numerical solution of initial value problems during the 1980’s, have actively continued research till now and proposed many fourth order RK methods, embedded methods, fifth order weighted mean methods and methods for parallel processors [49-58, 95-97, 120, 121, 145-150].
RK methods are being applied to determine numerical solutions for the problems, which are modeled as IVPs involving differential equations that arise in the fields of Science and Engineering. Though the RK method had been introduced at the turn of 20th century, research in this area is still very active and its applications are enormous. This is because of its nature of extending accuracy in the determination of approximate solutions and its flexibility.

Runge-Kutta methods have become very popular, both as computational techniques as well as subject for research. This method was derived by Runge about the year 1894 and extended by Kutta a few years later. They developed algorithms to solve differential equations efficiently and yet are the equivalent of approximating the exact solution by matching n terms of the Taylor series expansion.

The general p-stage Runge-Kutta method for solving an IVP

\[ y' = f(x, y) \quad (1.1) \]

with the initial condition \( y(x_0) = y_0 \) is defined by

\[ y_{n+1} = y_n + h \sum_{i=1}^{p} b_i k_i \quad (1.2) \]

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a. CARL DAVID TOLMÉ RUNGE, one of the most notable applied mathematicians of Germany, also known as a physicist through his investigations on spectral series, was one of the pioneers in the application of mathematical methods to the numerical treatment of technical problems. Runge was born in Bremen on the 30th August 1856 and spent his early childhood in Havanna. From 1876 to 1880 he studied first in Munich and then in Berlin, where he took his doctor's degree in 1880; he became an unsalaried lecturer at the University of Berlin in 1883 and was later, 1886, appointed as professor of mathematics in the Technische Hochschule, Hannover. From 1904 to 1924 he was professor of applied mathematics in Gottingen, where he died on the 3rd January, 1927

b. MARTIN WILHELM KUTTA, born on the 3rd November, 1867 in Pitschen (Upper Silesia), Germany, studied in Breslau from 1885 to 1890, then went to Munich, where he took his doctor's degree in 1901 and became an unsalaried lecturer in 1902. He spent 1898 – 1899 in Cambridge. In 1910 he was appointed to Aachen and in 1911 to Stuttgart as ordinary professor of mathematics (emeritus 1935). He died on the 25th December, 1944 in Fürstenfeldbruck (near Munich) Germany.
where
\[ k_1 = f \left( x_n + c_i \cdot h, y_n + h \sum_{j=1}^{p} a_{ij} k_i \right) \]  \hfill (1.3)

and
\[ c_i = \sum_{j=1}^{p} a_{ij}, \quad i = 1, 2, \ldots, p \]

with \( c \) and \( b \) are \( p \) dimensional vectors and \( A(a_{ij}) \) be the \( p \times p \) matrix. The Butcher array form is

\[
\begin{array}{ccccccccc}
0 & c_1 & a_{11} & c_2 & a_{21} & \cdots & c_p & a_{p1} & a_{p2} & \cdots & a_{p,p-1} \\
& b_1 & b_2 & b_3 & \cdots & b_{p-1} & b_p \\
\end{array}
\]  \hfill (1.4)

1.1 DISCUSSION OF LITERATURE

Ordinary differential equations are the principal form of mathematical model occurring in Science and Engineering, and, consequently, the numerical solution of differential equations is a very large area of study. Two classic textbooks, which reflect the state of knowledge before the widespread use of digital computers, are Collatz [38] and Milne [91]. Since 1960, some important text are in chronological order, Henrici [71]; Ceshino and Kuntzmann [31], Lapidus and Seinfeld [85], Gear [60], Lambert [83], Hall and Watt [69], Shampine and Watt [124, 125] and Hairer et al. [66, 67] most of them contain large bibliographies.

The text by Henrici [71] has become a classic account of Numerical solution of ODE's, including extensions and its applications and Gear [60] is a more modern account of all methods. A complete account up to 1970 of Runge-Kutta methods, their developments and error analysis, is given in Lapidus and Seinfeld [85].
Many textbooks, which deal with numerical analysis such as Scarborough [122], Hilderbrand [72], Atkinson [2], Conte and Boor [41] and Ralston and Wilf [111], present the Runge-Kutta methods with error control and automatic step-size selection.

Because of the creation of a number of automatic programs for solving differential equations, several empirical studies have been made to assess their performance and to make comparisons between programs. Two major projects have been presented: one by Hull et al. [77] and the other by Shampine and Watts [126]. It is clear from their work that programs must be compared, as well as methods, and also in 1991, Sharp [129] compared some RK pairs of order 4 through 8. The Runge-Kutta methods for the systems and the higher order IVPs are discussed in [64, 94-97, 126].

Butcher [17] studied Runge-Kutta methods in considerable detail and it is a centerpiece of his book, and he explained the stability and algebraic properties of Runge-Kutta methods. He also surveyed a number of questions and results concerning Runge-Kutta and general linear methods in [18].


Recently the numerical solution of system of IVPs of delay differential equations and its stability are studied by the following authors, Yang et al. [151], Hung [76], Ismail and Suleiman [81], Baker and Paul [5], Hu et al. [65] and Iserles [79].
The use of partitioned methods, for a given stiff and non-stiff subsystems, are presented and investigated for Runge-Kutta type methods by Weiner et al. [142]. Runge-Kutta methods for IVPs of periodic [3, 131], with oscillating solutions [20, 32], with rapidly varying right-hand sides [29] and for rigid body Lie-Poisson equations [48] have been discussed recently.

Many Runge-Kutta (RK) codes for the numerical solution of non-stiff initial value problems in ODEs are based on embedded pairs of RK formulae. The six stage RKF(4,5) pair due to Fehlberg proved to be very effective and based on this pair Shampine and Watts [126] designed a user oriented package DEPAC to solve ODE. The subroutine DVERK [78] produced by Hull et al. is based on a pair of formulae of orders 5 and 6 due to Verner [138]. For computations, which require higher accuracy, a pair of orders 7 and 8 of Fehlberg [59] has been widely used. Dormand and Prince [45, 46] have presented new pairs of RK formulae, which are superior in most respects to those currently in use. A new pair of embedded Runge-Kutta formulae of orders 5 and 6 was presented by Calvo et al. [22]. Bogacki and Shampine [13] derived a pair of explicit Runge-Kutta formulae of orders 4 and 5, which is significantly more efficient than the Fehlberg and Dormand-Prince [110] pairs. Papakostas and Tsitouras [106] also defined a new family of 6(5) Runge-Kutta pairs.

Among the large variety of methods available for the numerical solution of IVPs, one can distinguish between continuous and discrete methods. The class of explicit Runge-Kutta methods has traditionally belonged to the latter group. Recently, however, many authors have investigated continuous extensions of one-step methods; see Enright et al. [47], Horn [73], Shampine [127]. Brynjulf and Marino [28] presented an article on continuous explicit Runge-Kutta methods. Derr et al. [43] introduced a new method for derivation of continuous Runge-Kutta formulae. Some of these authors use the strategy of supplying an already existing
discrete RK method with an interpolant in order to obtain a continuous method with the desired accuracy and also Gladwell et al. [62] have discussed practical aspects of interpolation in Runge-Kutta codes.

Iserles and Norsett [80] created a theoretical framework for parallelisation of Runge-Kutta methods. Cong [39, 40] designed a explicit parallel Two-step Runge-Kutta Nyström methods for the special second order equation \( y''(x) = f(y(x)) \). It is observed that many researchers have contributed much about the concept of stability, error estimation and automatic step-size selection [5, 17, 21, 30, 42, 60, 63, 67, 69-71, 78, 81, 83, 85].

The classical fourth order Runge-Kutta method is based on the Arithmetic Mean (AM). In addition, the emergence of non-linear type of Runge-Kutta methods based on a variety of means such as Harmonic Mean (HaM) [120], Heronian Mean (HeM) [55], Contraharmonic Mean (CoM) [54], Root Mean square (RM) [147], Geometric Mean (GM) [49,119] and Centroidal Mean (CeM) [52] have been actively studied by Evans and his team of researchers. It is indeed Evans and his team of researchers who introduced a new dimension to the numerical solution of initial value problems during the 1980’s and have actively continued research till now and have proposed many fourth order embedded methods, fifth order weighted mean methods etc.

Wazwaz [141] have compared the modified third order RK formulae based on a variety of means. Yaakub and Evans [150] studied the RK methods based on different means as a starters for multi-step methods. Also they [148] implemented the RK method based on Contraharmonic Mean using Romberg extrapolation on a parallel computer. Evans and Yaakub [56, 149] introduced a new embedded RK (4, 4) method based on AM and CoM.
Yaakub and Evans presented a new four-stage fifth order RK method [145], a new weighted RK fifth order with 5 stages method [57, 58] and developed a new 3-stage 4th order RK for solving IVPs [146].

Murugesan et al., [95 - 97] have analyzed different second order systems, multivariable linear systems, especially non-linear singular system from fluid dynamics using extended RK methods based on AM, HaM and HeM.

The aim of this thesis is to approach the system of IVPs of linear, non-linear, stiff, singular time-invariant and time-varying systems by straight-forward extension of the fourth order RK methods based on a variety of means AM, CeM, HaM, HeM, CoM, GM and RM. In particular, our interest will be focused on the RK method based on CeM. Hence our results include some of the results obtained by Evans and his team. However, we would like to point out, that our approach differs essentially from those of Evans and his team of researchers, since we use a system of IVPs to derive the conclusions of the discussed RK methods.

1.2 CONTRIBUTIONS OF THIS THESIS

One of the contributions of this thesis is the extension of the fourth order RK methods based on a variety of means to solve a system of IVPs. Wazwaz [141] published a paper on modified Runge-Kutta formula based on a variety of means of third order. Evans and his team of researchers have derived a number of new fourth order RK formulae based on a variety of means. In all the papers, they have tested the methods using single IVPs and their efficiency has been established. Hence seven different real-life system of IVPs, like Robot arm control model, singular system of Electronic circuit, Voltera model of predator-prey oscillations, Dynamics of a gas absorber problem, etc., are studied using extended RK methods based on a
variety of means. In particular, the algorithm to solve the system of IVPs is given as a single structure for all the seven means discussed. Moreover, it is noted that stability analysis have been done, for all the proposed RK methods, and the area of stability regions have been compared and represented pictorially.

Possibly, the most important contribution of this thesis is the development of a new embedded RK method, based on AM and CeM with error control, which is denoted as RKACeM(4,4). This is presented in Chapter – 4 and it is based on the paper RK(4,4) derived by Evans and Yaaakub [56,149]. This new method is also compared with the well known methods like RK Fehlberg(4,5) and RK Merson methods.

Another contribution of this thesis is the extension of the fourth order RK method based on a variety of means to solve a system of second order IVPs directly. This is explained in Chapter – 5 and the main focus is given to RKCeM method with automatic step-size selection.

A further contribution, is the study on time-varying singular system via the extended RK methods based on AM and CeM and the STWS technique. Our research team made a remarkable attempt to develop the procedure of the time-invariant and time-varying STWS technique for solving system of second order IVPs directly without reducing to first order.

Further, we developed a new procedure to solve one dimensional heat flow problem by combining Rayleigh Ritz method, with the STWS technique and the discussed RK methods. In addition to this, we have improved the numerical solution for RLC smoothing circuit problem analyzed by Palanisamy and Arunachalam [102]. These two studies are the last, though not necessarily the least, contribution of this thesis.
1.3 A BRIEF SURVEY OF THE CHAPTERS

In Chapter II, several fourth order Runge-Kutta formulae based on Arithmetic Mean (AM), Centroidal Mean (CeM), Harmonic Mean (HaM), Geometric Mean (GM), Root Mean square (RM), Heronian Mean (HeM) and Contraharmonic Mean (CoM) are studied along with their error and stability region. The stability region has been represented pictorially depicting the superiority of the proposed RKCeM method.

In Chapter III, fourth order RK methods, based on a variety of means, have been extended to solve the system of linear and non-linear differential equations. The accuracies of the above new formulae are tested for seven major realistic problems existing in the fields of Science and Engineering. The investigation undertaken in this study reveals that the extended fourth order RK methods, on AM and CeM suit well for the systems of IVPs.

In Chapter IV, an attempt has been made, to develop an embedded RK method, based on the combination of AM and CeM which are both of order $p = 4$, and this combination is written as RKACeM(4,4). Different types of linear as well as non-linear IVPs have been analyzed by employing the proposed method and the results are compared with RK Fehlberg, RK Merson Methods and RK(4, 4) method developed by Yaakub and Evans. From the results and discussions, it is found that RKACeM(4, 4) is better than the method RK(4, 4), in terms of accuracy and time taken, and agree very well with RK Fehlberg and RK Merson methods.

In Chapter V, to solve second order differential equations, fourth order Runge-Kutta method based on Centroidal Mean has been extended. The effectiveness of this extended approach is tested for ten different second order systems of IVPs and compared with other RK methods. Here, an automatic step-size selection is made possible with the help of the error
estimate. Among the discussed problems, RK method based on Centroidal Mean gives best accuracy for five problems, and for the remaining five problems, it occupies second position in terms of accuracy whereas RK method based on AM, occupies the first position when compared to other RK methods based on HaM, HeM and CoM.

In Chapter VI, we consider the extended RK methods based on AM and CeM, and Single Term Walsh Series (STWS) technique. Singular time-varying systems are much more difficult to solve than time-invariant systems [75]. Three different practical problems are studied under the first order time-varying system. The first system is the state analysis of time-varying singular bilinear system, second is the observer design of time-varying singular system of transistor circuits and the third is the time-varying state-space system of electronic circuits. In the case of second order systems two problems are considered; of the two, one being the reduction of the first order system of transistor circuit to second order system which provides a greater accuracy, where execution time and storage space are minimized.

In the last Chapter VII, two practical problems are studied. The first is, one dimensional heat-flow problem and the other is RLC smoothing circuit. For the heat-flow problem, we introduced methods by combining Rayleigh-Ritz method with STWS, and Rayleigh-Ritz method with extended RK method based on Centroidal and Harmonic Mean. The discrete solutions obtained by the above mentioned methods are being compared with the exact solutions and also the discrete solutions using Laplace Transform and extended RK method based on AM. In addition, this chapter also presents an analysis of RLC smoothing circuits using STWS and extended RK method based on AM and CeM. The solution is obtained both in exact and discrete forms. The results are compared with the results obtained by Palanisamy and Arunachalam [102]. Here, it is suggested that when the output of a digital to analogue
converter is a staircase function, one has to introduce the initial condition at every sub-interval for the given range to achieve a greater accuracy in results.

The efficiency of the methods, discussed in every chapter, has been studied with respect to different aspects-like time, accuracy, error, etc. The algorithms of the discussed methods have been computerized using ‘C’ language [109] in order to obtain the results. All the programs are stored in a 3.5” disk under the directory ‘RK-7-MEANS’. The floppy disk is attached in the inner side of the back cover, and the program list is given in Appendix, chapterwise.

Consequent to this research work, the author has obtained some significant results in the following topics:

(i) A study on the stability region and error for the fourth order RK method based on a variety of means.

(ii) A comparison of extended Runge-Kutta formulae based on a variety of means to solve the system of IVPs.

(iii) A fourth order embedded Runge-Kutta RKACeM(4,4) method based on arithmetic and centroidal means with error control.

(iv) Numerical strategies for second order IVPs using fourth order Runge-Kutta method based on centroidal mean.

(v) Analysis of first and second order time-varying singular systems via extended RK methods and STWS technique.


(vii) Solution of RLC smoothing circuits using extended RK methods and STWS Technique.