RUNGE-KUTTA METHOD OF DIFFERENT ORDERS FOR NUMERICAL SOLUTION OF INITIAL VALUE PROBLEMS

1.1 Introduction

It is well known that the majority of differential equations in Science and Engineering can not be integrated analytically. So it becomes necessary to solve such equations numerically by approximation methods. There are a large number of approximation methods for solving the initial value problems and the boundary value problems. After the advent of high speed computers, the numerical methods for solving both ordinary and partial differential equations become more and more popular. Most of these methods are discussed in standard texts like Colatz (1966), Hildebrand (1974), Jain (1979), Fox (1962), Lapidus and Seinfeld (1971), Henrici (1962). Amongst the methods for the approximate numerical solution of the initial value problem

$$\frac{dy}{dt} = f(t, y)$$

$$y(t_0) = y_0 . \qquad (1.1.1)$$

the Runge-Kutta methods are most popular because of their accuracy and numerical stability. Here, our aim is to discuss this method with particular emphasis on some developed Runge-Kutta procedures, their computer programming and the numerical tests of those programs.

Carl David Tolmi Runge one of the most notable German Mathematician 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. E. Trefftz (1926) writes on him “If Runge succeeded in bringing the gap between mathematics and technology, his success was due to two characteristics, which mark a true applied mathematician, his profound mathematical knowledge …., and his unflagging energy in perfecting his methods with particular regard to their practical usefulness”.

Runge was born in Bremen on 30th, August, 1856 and spent his early childhood in Havana, where his father was in charge of administration of Danish Consulate. 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 3rd, January 1927. He also travelled to New York in 1909, where he was exchange Professor in the Columbia University for the winter semester. Prandtl (1927) writes "He was a kindly disposition, yet strongly independent of his opinions even to sever condemnations of that which appeared to him unfair and narrow minded. With regard to himself he was extremely modest".

Martin Wilhelm Kutta was born on 3rd November, 1867 in Pitschen, 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. He died on 28th December, 1944 in Furstenfeldbruck (near Munich) where he was staying with his brother.

The original method was devised first by Runge (1895) and developed mainly by Kutta (1901) and Heun (1900). In the next section we discuss briefly the derivation of the Runge-Kutta formulas of different orders.

1.2 Second Order Method

We discuss the initial value problem given by equation (1.1.1). The numerical solution of this equation is sought at

$$t_n = t_0 + nh, n = 1, 2, ... \quad (1.2.1)$$

where h is a fixed positive number and $t_n \in [t_0, b]$.

Let

$$\left.\begin{aligned} k_1 &= hf\,(t_n\ ,\ y_n) \\ k_2 &= hf\,(t_n + c_2 h,\ y_n + a_{21} k_1 \\ y_{n+1} &= y_n + w_1 k_1 + w_2 k_2 \end{aligned}\right\} \qquad [1.2.2]$$

where the parameters $c_2\,, a_{21}\,, w_1\,, w_2$ are so chosen that the approximate solution y_{n+1} at t_{n+1} is close to $y(t_{n+1})$. Now by Taylor series expansion,

$$y(t_{n+1}) = y(t_n + h)$$

$$= y(t_n) + hy'(t_n) + \frac{h^2}{2!} y''(t_n) + \cdots \qquad (1.2.3)$$

In view of equation (1.1.1),

$$y'' = f_t + ff_y$$

$$y''' = f_{tt} + ff_{ty} + f\,(f_{ty} + ff_{yy}) + f_y(f_t + ff_y)$$

$$= f_{tt} + 2\,ff_{ty} + f^{\,2} f_{yy} + f_y(f_t + ff_y)$$

$$y''' = f_{tt} + 2\,ff_{ty} + f_{yy} f^{\,2} + f_y(f_t + ff_y) \qquad (1.2.4)$$

Referring (1.2.2),

$$k_1 = hf\,(t_n, y_n)$$

$$k_2 = hf\,(t_n + c_2 h\ ,\ y_n + a_{21} hf_n)$$

$$= h[\,f\,(t_n\,, y_n) + (c_2 hf_t + a_{21}\,hf_n\ f_y)]\ + \frac{(c_2 h + a_{21} h)^2}{2!}\left(\frac{\partial}{\partial t}\right)^2 f + \cdots$$

$$= hf_n + h^2\left(c_2\,f_t + a_{21} f_n\,f_y\right) + \frac{1}{2} h^3\left(c_2^2\ f_{tt} + 2c_2 a_{21}\ f_n\,f_{ty} + a_{21}^2\ f_n^{\,2}\ f_{yy}\right) + \cdots \quad (1.2.5)$$

Now putting the values of k_1 and k_2 from (1.2.5) in (1.2.2) we get

$$y_{n+1} = y_n + w_1 h f_n + w_2 \Big[h f_n + h^2 (c_2 f_t + a_{21} f_n f_y)$$

$$+ \frac{1}{2} h^3 (c_2^2 f_{tt} + 2 c_2 a_{21} f_n f_{ty} + a_{21}^2 f_n^2 f_{yy}) \Big]$$

$$= y_n + (w_1 + w_2) h f_n + h^2 (w_2 c_2 f_t + w_2 a_{21} f_n f_y)$$

$$+ \frac{1}{2} h^3 w_2 \left(c_2^2 f_{tt} + 2 c_2 a_{21} f_n f_{ty} + a_{21}^2 f_n^2 f_{yy} \right) + \ldots \qquad (1.2.6)$$

Now matching the coefficients of power of h of (1.2.6) with (1.2.3), we get

$$w_1 + w_2 = 1$$

$$w_2 c_2 = \frac{1}{2}$$

$$a_{21} w_2 = \frac{1}{2}$$

$$\Rightarrow c_2 = a_{21} \ , \ w_2 = \frac{1}{2} c_2 \ , \ w_1 = 1 - \frac{1}{2 c_2} \qquad (1.2.7)$$

Using (1.2.7) in (1.2.6), we have

$$y_{n+1} = y_n + h f_n + \frac{h^2}{2} (f_t + f_n f_y) + \frac{c_2 h^3}{4} (f_{tt} + 2 f_n f_{ty} + f_n^2 f_{yy}) + \cdots \qquad (1.2.8)$$

For getting the truncation error T_n, let us subtract (1.2.8) from (1.2.3),

$$T_n = h^3 \left[\left(\frac{1}{6} - \frac{c_2}{4} \right) \left(f_{tt} + 2 f_n f_{ty} + f_n^2 f_{yy} \right) + \frac{1}{6} f_y \left(f_t + f_n f_y \right) \right] + \cdots \qquad (1.2.9)$$

Now taking different values for the parameters c_2, a_{21}, w_1, w_2 we can get different second order Runge-Kutta formulas. These are referred to as the improved tangent method or improved polygon method (cf. Collatz (1966), Euler-Cauchy method (cf. Hildebrand (1974) and the optimal method (cf. Jain (1979)).

From improved tangent method we have taken

$$\begin{aligned} c_2 &= 0.5 \\ w_1 &= 0 \\ w_2 &= 1 \end{aligned} \tag{1.2.10}$$

For Euler-Cauchy method we have considered

$$\begin{aligned} c_2 &= 1 \\ w_1 &= 0.5 \\ w_2 &= 0.5 \end{aligned} \tag{1.2.11}$$

Similarly for optimal method or Heun method, we have

$$\begin{aligned} c_2 &= \frac{2}{3} \\ w_1 &= \frac{1}{4} \\ w_2 &= \frac{3}{4} \end{aligned} \tag{1.2.12}$$

1.3 Third Order Method

As in case of second order methods, here we have to define three k's to get a third order method.

Let us define

$$k_1 = hf(t_n, y_n)$$

$$k_2 = hf(t_n + c_2 h, y_n + a_{21} k_1)$$

$$k_3 = hf\,(t_n + c_3 h, y_n + a_{31} k_1 + a_{32}\, k_2) \tag{1.3.1}$$

$$y_{n+1} = y_n + w_1 k_1 + w_2 k_2 + w_3 k_3$$

Assuming all the conditions of (1.2.1) are also satisfied.

Now expanding $y(t_{n+1}) = y(t_n + h)$ by Taylor's series as (1.2.3) and also expanding k_2, k_3 by Taylor's series for several variables we get y_{n+1}. Comparing the coefficients of the powers of h in both the series, we get the relationship among the parameters $c_2, c_3, a_{21}, a_{31}, a_{32}, w_1, w_2, w_3$.

$$a_{21} = c_2$$

$$a_{31} + a_{32} = c_3$$

$$c_2 w_2 + c_3 w_3 = \frac{1}{2} \tag{1.3.2}$$

$$c_2^2 w_2 + c_3^2 w_3 = \frac{1}{3}$$

$$w_1 + w_2 + w_3 = 1$$

$$c_2\, a_{32}\, w_3 = \frac{1}{6}.$$

In (1.3.2), we are having six equations for eight variables. So assigning different values to different values to different variables, we get formulas for third order Runge-Kutta method. For the present discussion, we have considered four third order Runge-Kutta formulas. Those are referred to as Nystrom method (cf. Nystrom, (1925), Heun method (cf. Heun, (1900)), Classical method (cf. Hildebrand, (1974), Nearly-Optimal method (cf. Jain, (1979)).

These methods are compactly given by means of the following tables. Let the parameters be arranged as follows.

Table - 1.1

c_2	a_{21}		
c_3	a_{31}	a_{32}	
	w_1	w_2	w_3

In view of Table – 1.1, for Nystrom method we have

Table - 1.2

$\frac{2}{3}$	$\frac{2}{3}$		
$\frac{2}{3}$	0	$\frac{2}{3}$	
	$\frac{2}{8}$	$\frac{3}{8}$	$\frac{3}{8}$

For Nearly-optimal method, the parameters are,

Table - 1.3

$\frac{1}{2}$	$\frac{1}{2}$		
$\frac{3}{4}$	0	$\frac{3}{4}$	

	$\frac{2}{9}$	$\frac{3}{9}$	$\frac{4}{9}$

Similarly for classical method, we have

Table - 1.4

$\frac{1}{2}$	$\frac{1}{2}$		
1	-1	2	
	$\frac{1}{6}$	$\frac{4}{6}$	$\frac{1}{6}$

For Heun method, we have assigned,

Table - 1.5

$\frac{1}{3}$	$\frac{1}{3}$		
$\frac{2}{3}$	0	$\frac{2}{3}$	
	$\frac{1}{4}$	0	$\frac{3}{4}$

1.4 Fourth Order Methods

As in case of Second order and Third order methods, here we are going to discuss the fourth order Runge-Kutta methods. In this case four k's will be used for evaluation of y_{n+1}. With the help, of these k's we can manage to get fourth order Runge-Kutta methods. Let us define.

$$k_1 = hf\,(t_n, y_n)$$

$$k_2 = hf\,(t_n + c_2 h, y_n + a_{21} k_1) \tag{1.4.1}$$

$$k_3 = hf\,(t_n\, c_3 h, y_n + a_{31} k_1 + a_{32} k_2)$$

$$k_4 = hf\,(t_n + c_4 h,\; y_n + a_{41} k_1 + a_{42} k_2 + a_{43} k_3)$$

$$y_{n+1} = y_n + w_1 k_1 + w_2 k_2 + w_3 k_3 + w_4 k_4$$

where $c_2, c_3, c_4, a_{21}, a_{31}, a_{32}, a_{41}, a_{42}, a_{43}, w_1, w_2, w_3, w_4$ are parameters. Details of the derivations of the conditions are relations that exist among the parameters c_2, c_3, c_4, $a_{21}, a_{31}, a_{32}, a_{41}, a_{42}, a_{43}, w_1, w_2, w_3, w_4$ is exactly similar to that in case of second and third order methods. For the present we shall discuss three different fourth order Runge-Kutta methods. Those are classical methods (cf. Hildebrand, (1974), Kutta method (cf. Kutta, (1901), Gill method (cf. Gill, (1951)). As in the previous section, we shall represent the values of the parameters for different fourth order Runge-Kutta formulas by the table given below.

Table - 1.6

c_2	a_{21}			
c_3	a_{31}	a_{32}		
c_4	a_{41}	a_{42}	a_{43}	
	w_1	w_2	w_3	w_4

Like Table 1.6, we have for Classical method,

Table - 1.7

$\frac{1}{2}$	$\frac{1}{2}$			
$\frac{1}{2}$	0	$\frac{1}{2}$		
1	0	0	1	
	$\frac{1}{6}$	$\frac{2}{6}$	$\frac{2}{6}$	$\frac{1}{6}$

Similarly for Kutta method, we have taken,

Table - 1.8

$\frac{1}{3}$	$\frac{1}{3}$			
$\frac{2}{3}$	$-\frac{1}{3}$	1		
1	1	-1	1	
	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$

Also for Gill method, we considered,

Table - 1.9

$\frac{1}{2}$	$\frac{1}{2}$			
$\frac{1}{2}$	$\frac{(\sqrt{2}-1)}{2}$	$\frac{(2-\sqrt{2})}{2}$		
1	0	$\frac{-\sqrt{2}}{2}$	$1+\frac{\sqrt{2}}{2}$	
	$\frac{1}{6}$	$\frac{(2-\sqrt{2})}{6}$	$\frac{(2+\sqrt{2})}{6}$	$\frac{1}{6}$

1.5 Fifth Order Method

In this Section we are going to discuss the fifth order Runge-Kutta method, which will be used to approximate the solution of the initial value problem (1.1.1). Similar to the second, third and fourth order methods, here we are having six k's, for which we are able to get fifth order Runge-Kutta formula. But in this case we are having six weights i.e. w_i's, unlike in previous cases two, three and four weights in second, third and fourth order methods. So these fifth order methods are also represented as (5,6) which means order five and six weights and k's.

Let us define

$$k_1 = hf\,(t_n, y_n)$$

$$k_i = hf\,(t_n + c_i h, y_n + \sum_{j=1}^{i-1} a_{ij} k_j) \quad \text{for} \quad 2 \le i \le 6 \qquad (1.5.1)$$

$$y_{n+1} = y_n + \sum_{i=1}^{6} w_i k_i$$

where c_i, a_{ij}, w_i are parameters.

The details of the derivations for the relations between these parameters is exactly same as that of second and third order methods. In this case, we shall get sixteen equations for twenty one unknowns. So we get five free parameters. Because of this, the freedom of parameter choice leads to a wide set of possible Runge-Kutta formulae. Therefore, without considering all the fifth order formulas, we have considered Nystrom method (cf. Nysrom, (1925)) as it is the most well-known and Lawson method (cf. Lawson, (1966)) as it has an extended region of stability. As in previous sections, here we shall denote the various fifth order formula by table.

Table - 1.10

c_2	a_{21}					
c_3	a_{31}	a_{32}				
c_4	a_{41}	a_{42}	a_{43}			
c_5	a_{51}	a_{52}	a_{53}	a_{54}		
c_6	a_{61}	a_{62}	a_{63}	a_{64}	a_{65}	
	w_1	w_2	w_3	w_4	w_5	w_6

Keeping in mind (1.5.2), for Nystrom method, we have

Table - 1.11

$\frac{1}{3}$	$\frac{1}{3}$					
$\frac{2}{5}$	$\frac{4}{25}$	$\frac{6}{25}$				
1	$\frac{1}{4}$	$-\frac{12}{4}$	$\frac{15}{4}$			
$\frac{2}{3}$	$\frac{6}{81}$	$\frac{90}{81}$	$-\frac{50}{81}$	$\frac{8}{81}$		
$\frac{4}{5}$	$\frac{6}{75}$	$\frac{36}{75}$	$\frac{10}{75}$	$\frac{8}{75}$	0	
	$\frac{23}{192}$	0	$\frac{125}{192}$	0	$-\frac{81}{192}$	$\frac{125}{192}$

In view of (1.5.2), the Lawson formula is

Table - 1.12

$\frac{1}{2}$	$\frac{1}{2}$					
$\frac{1}{4}$	$\frac{3}{16}$	$\frac{1}{16}$				
$\frac{1}{2}$	0	0	$\frac{1}{2}$			
$\frac{3}{4}$	0	$-\frac{3}{16}$	$\frac{6}{16}$	$\frac{9}{16}$		
1	$\frac{1}{7}$	$\frac{4}{7}$	$\frac{6}{7}$	$-\frac{12}{7}$	$\frac{8}{7}$	
	$\frac{7}{90}$	0	$\frac{32}{90}$	$\frac{12}{90}$	$\frac{32}{90}$	$\frac{7}{90}$

1.6 Sixth Order Methods

Quite similar to the second, third, fourth, fifth order Runge-Kutta methods, we shall discuss sixth order Runge-Kutta methods in this section. For these methods, we shall have to deal with seven or eight k's with the same number of weights.

Let us define,

$$k_1 = hf(t_n, y_n)$$

$$k_i = hf(t_n + c_i h, y_n + \sum_{j=1}^{l} k_{ij} a_{ij}) \quad 2 \le i \le l \tag{1.6.1}$$

$$y_{n+1} = y_n + \sum_{j=1}^{l} w_j k_j$$

where w_j, a_{ij}, c_i are parameters.

Our aim is to establish the relationship among these parameters. We proceed to find it exactly similar as (1.2.3)- (1.2.6). Here also we shall get a lot of sixth order Runge-Kutta formulas. But only two formulas due to Huta (cf. Butcher, (1963)) and Bucher (cf. Butcher, (1964)) are taken into consideration. Huta's formula is of type (6,8), whereas Butcher formula is of type (6,7). Hence in (1.6.1), l will be equal to 8 for Huta and 7 for Butcher formula. As usual we shall refer to those formula by a table to be mentioned.

For Butcher method, we have

Table - 1.13

$\frac{1}{3}$	$\frac{1}{3}$						
$\frac{2}{3}$	0	$\frac{2}{3}$					
$\frac{1}{3}$	$\frac{1}{12}$	$\frac{1}{3}$	$-\frac{1}{12}$				
$\frac{1}{2}$	$-\frac{1}{16}$	$\frac{9}{8}$	$-\frac{3}{16}$	$-\frac{3}{8}$			
$\frac{1}{2}$	0	$\frac{9}{8}$	$-\frac{3}{8}$	$-\frac{3}{4}$	$\frac{1}{2}$		
1	$\frac{9}{44}$	$-\frac{9}{11}$	$\frac{63}{44}$	$\frac{18}{11}$	0	$-\frac{16}{11}$	
	$\frac{11}{120}$	0	$\frac{27}{40}$	$\frac{27}{40}$	$-\frac{4}{15}$	$-\frac{4}{15}$	$\frac{11}{120}$

For Huta method, we have

Table - 1.14

$\frac{1}{9}$	$\frac{1}{9}$							
$\frac{1}{6}$	$\frac{1}{24}$	$\frac{3}{24}$						
$\frac{1}{3}$	$\frac{1}{6}$	$-\frac{3}{6}$	$\frac{4}{6}$					
$\frac{1}{2}$	$-\frac{5}{8}$	$\frac{27}{8}$	$-\frac{24}{8}$	$\frac{6}{8}$				
$\frac{2}{3}$	$\frac{221}{9}$	$-\frac{981}{9}$	$\frac{867}{9}$	$-\frac{102}{9}$	$\frac{1}{9}$			
$\frac{5}{6}$	$-\frac{183}{48}$	$\frac{678}{48}$	$-\frac{472}{48}$	$-\frac{66}{48}$	$\frac{80}{48}$	$\frac{3}{48}$		
1	$\frac{716}{82}$	$-\frac{2079}{82}$	$\frac{1002}{82}$	$\frac{834}{82}$	$-\frac{454}{82}$	$-\frac{9}{82}$	$\frac{72}{82}$	
	$\frac{41}{840}$	0	$\frac{216}{40}$	$\frac{27}{840}$	$\frac{272}{840}$	$\frac{27}{840}$	$\frac{216}{840}$	$\frac{41}{840}$

1.7 Truncation Error

In this Section, we discuss the truncation T_n associated with the approximation by Runge-Kutta method.

For the second order method, it is done in the following way. Subtracting equation (1.2.8) from equation (1.2.3), we get after simplification,

$$T_n = h^3\left[\left(\frac{1}{6}-\frac{c_2}{4}\right)\left(f_{tt}+2f_n f_{ty}+f_n^2 f_{yy}\right)+\frac{1}{6}f_y\left(f_t+f_n f_y\right)\right]$$

$$= h^3\left[\frac{1}{6}-\left(\frac{c_2}{4}\right)\right]D^2 f+\frac{h^3}{6}f_y Df$$

$$= O(h^3). \qquad (1.7.1)$$

Similarly for third order Runge-Kutta methods,

$$T_n = \left(\frac{h^4}{4!}\right)\left\{\left[1-4\left(c_2^3 w_2+c_3^3 w_3\right)\right]D^3 f+\left(1-12c_2^2 a_{32}w_3\right)f_y D^2 f\right.$$

$$\left.+\left(3-24c_2c_3w_3\right)Df\,Df_y+f_y^2\,Df\right\}$$

$$= O(h^4) \qquad (1.7.2)$$

In the same manner, we have in case of fourth, fifth and sixth order formulas,

$$\begin{aligned} T_n &= O(h^5)\\ T_n &= O(h^6)\\ T_n &= O(h^7) \end{aligned} \qquad (1.7.3)$$

In general, it is noted that the truncation error in case of *n*th order Runge-Kutta formula is given by $T_n = O(h^{n+1})$.

1.8 Program and Software Discussion

The program designed for Runge-Kutta methods is written in FORTRAN language. It is to note that the programs written in FORTRAN are in double precision So in single precision, we get the result correct upto sixteen significant places, whereas in double precision we get up to thirty two significant digits.

According to the design of the program, the user should input the initial point (*T*), the point where the approximate solution of the problem is sought (*PF*), step length (*H*) to be used. Also before running the program, the function *F*(*T*,*X*) should be incorporated in the desired form. Again care should be taken not to include the singular points of the f unction *F*(*T*,*X*). If the exact solution is not known, then the statements containing *R*(*T*) should be deleted in the program. For each order of the Runge-Kutta methods, separate subroutines are constructed to enable the user to have any or all of the methods. The second, third, fourth, fifth, and sixth order methods are contained in sub-routines RK2, RK3, RK4, RK5, RK6 respectively. The subroutine HEAD has only the role of printing the headings.

☞ [PROGRAM]

1.9 Numerical Experiment

For numerical verification of the different Runge-Kutta methods discussed and for the testing of the programs done, the following initial value problems (I.V.P.) is considered,

$$\frac{dy}{dt} = t + x \tag{1.9.1}$$

$$y(0) = 1.0 \tag{1.9.2}$$

For implementation of the programs framed in FORTRAN, the above I.V.P. is considered.