CHAPTER - I

INTRODUCTION

1.1 INITIAL VALUE PROBLEMS

Many Scientific and Engineering problems are reduced to Initial Value Problems associated with Ordinary Differential Equations. In many cases, it is difficult to find an exact analytical solution of these problems. With the advent of high speed electronic digital computers, derivation of suitable computational methods have been the subject of investigations in recent years.

An initial value problem of a single first order differential equation can be defined as

$$y' = f(x,y),\ y(x_0) = y_0 \qquad (1.1)$$

where $y' = \frac{dy}{dx}$.

The existence and uniqueness of the solution of the initial value problem (1.1) is guaranteed by the following theorem.

Theorem 1.1 If $f(x,y)$ satisfies the following conditions :

i) $f(x,y)$ is a continuous real valued function, defined in some domain D of the xy- plane where D is given by

$$D = \{ (x,y) \mid a \leq x \leq b, \ -\infty < y < \infty \} \text{ and}$$

ii) it satisfies the Lipschitz conditions, that is there exists a constant L such that, for every pair of points (x,y) and (x,y^*) lying in D,

$$| f(x,y) - f(x,y^*) | \leq L | y - y^* |, \qquad (1.2)$$

where L is called the Lipschitz constant and is defined as

$$L = \sup_{(x,y) \in D} \left| \frac{\partial f}{\partial y} \right|, \qquad (1.3)$$

then for any y_0, there exists a unique solution $y(x)$ of the initial value problem (1.1) for $x \in [a,b]$.

In most cases, we generally face, not with a single differential equation of the form (1.1) but with a set of simultaneous first order equations or a single equation of high order. The general non-linear differential equation of order can be written as

$$F(x, y, y', \ldots, y^{(m-1)}, y^{(m)}) = 0,$$

or, $$y^{(m)}(x) = f(x, y, y', \ldots, y^{(m-1)}). \qquad (1.4)$$

As equation (1.4) can be reduced to a system of m simultaneous first order differential equations, in general, we may write an initial value problem for a first order system as

$$\frac{dy_i}{dx} = y_i'(x) = f_i(x, y_1, y_2, \ldots, y_m),$$
$$y_i(x_0) = y_{i0}, \quad i = 1,2,\ldots m. \tag{1.5}$$

In vector notation (1.5) can be written as

$$\frac{d\underline{Y}}{dx} = \underline{Y}' = \underline{f}(x,\underline{Y}), \ \underline{Y}(x_0) = \underline{Y}_0 , \tag{1.6}$$

where,

$$\underline{Y} = [y_1, y_2, \ldots, y_m]^T,$$
$$\underline{f} = [f_1, f_2, \ldots, f_m]^T,$$
$$\underline{Y}_0 = [y_{10}, y_{20}, \ldots, y_{m0}]^T.$$

If the equation (1.6) is independent of x, then it is called autonomous, otherwise it is called nonautonomous. It can be noted here that from the numerical point of view, it is advantageous to consider a set of simultaneous equations rather than a single equation of high order.

Now, for the existence of the solution of the system (1.6), the domain D and the condition (1.2) of Theorem 1.1 can respectively be replaced by

$$D = \{ (x,\underline{Y}) \mid \ a \le x \le b, \ -\infty < \underline{Y} < \infty \},$$

and

$$\|f(x,\underline{y}) - f(x,\underline{y}^*)\| \leq L \|\underline{y} - \underline{y}^*\|,$$

where, $(x,\underline{y})$, $(x,\underline{y}^*) \in D$, $\|.\|$ denotes the vector norm and L is defined as

$$L = \sup_{(x,\underline{y})\in D} \|\frac{\partial \underline{f}}{\partial \underline{y}}\|,$$

where, $\frac{\partial \underline{f}}{\partial \underline{y}}$ is the Jacobian of $\underline{f}$ with respect to $\underline{y}$.

1.2 SINGLE STEP METHODS FOR SOLVING INITIAL VALUE PROBLEMS

1.2.1 Taylor Series Methods

When f(x,y) in (1.1) is sufficiently differentiable with respect to either x or y, then the simplest way of advancing the solution from the point x_n to x_{n+1} can be given by the Taylor series expansion as

$$y(x_{n+1}) = y(x_n) + hy'(x_n) + \frac{h^2}{2!} y''(x_n) + \ldots + \frac{h^k}{k!} y^{(k)}(x_n) + R_{k+1}, \quad x_n < \theta < x_{n+1}, \qquad (1.7)$$

where, $x_n = x_0 + nh$, h being the steplength used.

Neglecting the remainder term R_{k+1} in (1.7), the k-th order Taylor series method can be given as

$$y_{n+1} = y_n + hy_n' + \frac{h^2}{2!} y_n'' + \ldots + \frac{h^k}{k!} y_n^{(k)}, \quad n = 0,1,\ldots, N-1, \qquad (1.8)$$

where, $N = (b - a)/h$.

For some systems (linear) of differential equations, the Taylor series method may be used quite efficiently. However, unless the functions in the system are very simple, the higher order derivatives of $f(x,y)$ become increasingly complex which makes the Taylor series method completely unsuitable on high speed computers for general integration purposes. But Taylor series method will prove more effective than other methods of numerical integration for a certain class of systems where the simultaneous computation of all derivatives require a relatively small number of arithmatic operations. With recent developments in software, the automatic generation of algebraic expression for the derivatives of $f(x,y)$ will help the Taylor series method to be more widely used in future, [cf. Barton, Willers and Zahar (1971)]. An automatic integration programme based on the Taylor series method for solving initial value problems can also be found in Gibbons (1960).

1.2.2 Runge-Kutta Methods

These are single-step methods and do not require the higher order derivatives of $f(x,y)$ as in the Taylor series method. A general form of ν-stage Runge-Kutta method is usually written as

$$y_{n+1} = y_n + \sum_{i=1}^{\nu} \omega_i k_i , \qquad (1.9)$$

where,

$$k_i = hf(x_n + c_i h,\ y_n + \sum_{j=1}^{i-1} a_{ij} k_j) , \qquad (1.10)$$

$$i = 1,2,\ldots, \nu.$$

The parameters ω_i's, c_i's and a_{ij}'s are determined by satisfying (1.9) with the Taylor series expansion of as high an order as possible.

The 4-stage Runge-Kutta method of order four is widely used in practice with considerable success. The modified form of Runge-Kutta methods discussed by Blum (1962), Fype (1966), Gill (1951) have some advantages over the classical Runge-Kutta methods in respect of storage requirements in computer implementation. Runge-Kutta methods of various order have been studied by Butcher (1964a, 1965a), Luther (1966, 1968), Luther and Konen (1965), Roser (1967) and Shanks (1966). Runge-Kutta methods with minimum error have been described by Hull and Johnston (1964), King (1966), Ralston (1962). Methods discussed by King (1966) can be expected to provide increase in local accuracy for the initial value problems for which f(x,y), is independent of the dependent variable y. Runge-Kutta methods of order five and six with extended region of stability which have been studied by Lawson (1966, 1967) reduce the total number of function evaluation over a given interval of integration for the problems for which the condition of stability, rather than local accuracy is taken into consideration. More recently Day and Murthy (1981) have developed two classes of explicit generalized Runge-Kutta processes of which one class requires an accurate evaluation of the Jacobian at every step where as the other class requires less number of Jacobian evaluations per step and have shown that these methods are suitable for the integration of non-stiff systems of ordinary differential equations.

Fehlberg's work

Definition 1.1 The linear multistep method (1.11) is said to be of order q if it is exact for all monomials $y(x) = x^m$ $(m = 0,1,\ldots,q)$ and is not exact for $y(x) = x^{q+1}$.

Definition 1.2 The linear multistep method (1.11) is said to be consistent if it is atleast of order one i.e., $q \geq 1$.

Defining the first and second characteristic polynomials $\rho(r)$ and $\sigma(r)$ as

$$\rho(r) = -r^k + \sum_{j=1}^{k} a_k r^{k-j} ,$$
$$\sigma(r) = \sum_{j=o}^{k} b_o r^{k-j} , \tag{1.12}$$

having no common factor, the consistency condition for (1.11) can be shown to be equivalent to

$$\rho(1) = 0, \quad \frac{d\rho(r)}{dr}\Big|_{r=1} = \sigma(1). \tag{1.13}$$

The implication of (1.13) in that the first characteristic polynomial of (1.12) should have a root at $r = 1$ in order to have a consistent linear multistep method.

1.3.2 Truncation Error, Stability and Convergence

In the numerical integration of the initial value problem (1.1) one should be concerned with the truncation error and the numerical instability which may occur as, one actually approximates

the differential equation by a difference equation which is solved in a step by step process. Further, one should study the convergence of the generated difference scheme. By convergence we mean that the solution of the difference equation approaches the true solution as the step-size approaches zero. The concept of stability is associated with the propagation of errors of the numerical methods as the calculations progress with a finite interval size. This problem of instability arises because in most instances the difference equation is of a higher order than the original differential equation and possesses extraneous (spurious) solutions which do not vanish even in the limits as the step-size approaches zero.

TRUNCATION ERROR : This occurs due to the use of numerical technique that gives an approximate solution rather than the exact solution. Hence the truncation error is usually defined as the difference between the true value and the approximate value of the solution.

LOCAL TRUNCATION ERROR : This specifies the error in the solution at a single step in the process of numerical integration. For a method of order q, the local truncation error is usually given by

$$T(x,h) = c_{q+1}\, h^{q+1}\, y^{(q+1)}(\xi), \qquad (1.14)$$

where, c_{q+1} is the error constant.

ACCUMULATED TRUNCATION ERROR : Consideration of this error is extremely important in choosing a method. It is concerned with the propagation of the local truncation error as the integration proceeds.

We state the following lemmas in respect of the stability and convergence of any integration scheme of type (1.11) [Henrici (1962)].

Lemma 1.1 The method (1.11) is said to be zero-stable if no root of the first characteristic polynomial $\rho(r)$ has modulus greater than one and if every root with modulus one is simple.

Lemma 1.2 The necessary and sufficient conditions for the method (1.11) to be convergent are that it be consistent and zero-stable.

ATTAINABLE ORDER OF MULTISTEP METHODS : We can expect the highest order of a k-step method as 2k-1 if it is explicit and 2k if it is implicit. But, in general, the condition of zero-stability restricts the attainable maximal orders of a k-step methods as stated in the following theorem due to Dahlquist (1956). Which is as follows :

Theorem 1.2 No zero stable linear multistep method of step number k can have an order exceeding k+1 when k is odd or exceeding k+2 when k is even.

1.3.3 Weak Stability Theory of Linear Multistep Methods

From the condition of zero-stability, we are generally concerned with the nature of the solution as the step-size $h \longrightarrow 0$. But if we consider the case where the step-size h is strictly positive (i.e., $h > 0$), the study of absolute stability properties of a linear multistep method is important. In order to study this, we generally consider the scalar test equations

$$\frac{dy}{dx} = \lambda y , \tag{1.15}$$

where, we assume that λ is a complex constant with negative real part for which equation (1.15) is inherently stable for all initial conditions. Consequently, we have the stability polynomial, associated with the linear multistep method (1.11), as

$$\pi(r, \bar{h}) = \rho(r) + \bar{h}\, \sigma(r) = 0 , \tag{1.16}$$

where,

$$\bar{h} = \lambda h. \tag{1.17}$$

Definition 1.3 (Absolute stability) :

The linear multistep method (1.11) is said to be absolutely stable for a given value of $\bar{h}$ if, for that value of $\bar{h}$, all the roots r_j of the stability polynomial (1.16) satisfy $| r_j | < 1$ for all $j = 1,2,\ldots, k$.

Definition 1.4 (Interval of absolute stability) :

An interval (α, β) of the real line is said to be an interval of absolute stability if the method is absolutely stable for all $\bar{h} \in (\alpha, \beta)$.

The following points may be noted from the weak stability theory of linear multistep methods.

(i) Every consistent zero-stable linear multistep method is absolutely unstable for small positive values of $\bar{h}$.

(ii) If all the spurious roots of the first characteristics polynomial $\rho(r)$ lie strictly inside the unit circle then, the method has a non-vanishing interval of absolute stability.

(iii) If all the spurious roots are situated at the origin then, the interval of absolute stability is substantial.

If the required solution of linear multistep method decays faster than one of its spurious solution then, the error grows as integration proceeds. In this case, we usually, impose the condition of 'relative stability' originally proposed by Hull and Newbery (1962) which ensures that the spurious solutions decay faster than the required solution.

Definition 1.5 (Relative stability) : The linear multistep method (1.11) is said to be relatively stable for a given $\bar{h}$ if, for that value of $\bar{h}$, the roots r_j of (1.16) satisfy $|r_j| < |r_1|$ for $j = 2, \ldots, k$.

Definition 1.6 (Interval of relative stability) : An intefval (α, β) of the real line is said to be an interval of relative stability if the method is relatively stable for all values of $\bar{h} \in (\alpha, \beta)$.

The advantage of the multistep method is that in predictor-corrector mode, they provide an automatic error estimate at each step of integration so that one can select an optimum value of step length h for a required accuracy. In some cases, they may also reduce the computing time as the predictor-corrector methods require less number of function evaluations compared to that of Runge-Kutta methods.

For a non-stiff differential equation, Enright and Hull (1976) suggested that Runge-Kutta-Fehlberg methods and extra-polation methods are suitable if the derivative evaluations are relatively inexpensive. However, if the equations to be solved are many and the derivative evaluations are expensive, linear multistep methods (in PECE mode) are practically preferable because of the advantage in function evaluations per integration step. It is also seem from the literature that Runge-Kutta methods generally do not exibit any numerical instability for a sufficiently small step-size being used whereas Multistep Methods may in some cases be unstable for all values of step size and in other cases for a range of values of step-size.

Multistep Methods based on both numerical integration formulas and differentiation formulas have been described in detail by Henrici (1962). Multistep Methods based on polynomial approximation have also been discussed by Nordsieck (1962), Skeel (1979), Wallace and Gupta (1973). Multistep Methods with extendend region of stability and minimum truncation error have been discussed by Crane and Klopfenstein (1965), Hull (1967), Hull and Newbery (1961, 1962), Rahme (1969), Rodabaugh and Thompson (1978), Krough (1966) and Schoen (1971). The stability characteristics of multistep methods have been analysed by Brown et al. (1965), Chase (1962), Distefano (1968), Hall (1967), Iyenger and Jain (1974), Stetter (1965a, 1965b), and Rodabaugh (1970). The comparison of numerical methods for non-stiff ordinary differential equations have been made by Enright and Hull (1976), Hull et. al (1972), Krough (1973). Shampine

1.4 MODIFIED LINEAR MULTISTEP FORMULAS : HYBRID METHODS

The restriction on the condition of zero-stability given in Theorem 1.2 was circumvented by the introduction of modified linear multistep formulas, simultaneously proposed by Gragg and Stetter (1964), Butcher (1965b), Gear (1965a) by introducing one more function evaluation at an off-step point. They have shown that the possible order of a k-step method may be 2k or more. Again these modified k-step methods have been extended to two and an arbitrary number of off-step points by Brush et. al. (1967), Butcher (1967) and Lyche (1969). The modified k-step

method with ν slopes in the interval (x_n, x_{n+1}) can be defined as

$$y_{n+1} = \sum_{j=1}^{k} a_j y_{n+1-j} + h \sum_{j=0}^{k} b_j f_{n+1-j} + h \sum_{j=1}^{\nu} c_j f_{n+\theta_j}, \quad (1.18)$$

where a_j's, b_j's, c_j's and θ_j's are $2k+2\nu+1$ arbitrary parameters and $\theta_j \in (0,1)$ for $j = 1,2,\ldots,\nu$. The formula (1.18) is called an explicit hybrid method if $b_0 = 0$; otherwise it is called an implicit hybrid method. The conditions for consistency, stability and convergence of (1.18) are analogous to that of linear multi-step method (1.11).

When (1.18) is used in predictor-corrector mode, Kohfeld and Thompson (1967) pointed out that unless one uses an off-step point in the predictor formula the truncation error may be so large that the accuracy of the corrector will be largely lost. If the scheme (1.18) is used in PECE mode then its maximal order is $2k+2$ (one less if it is explicit) for $k \leq 4$ due to Gragg and Stetter (1964) and for $k \leq 6$ ($k \leq 4$ for explicit) due to Kohfeld and Thompson (1967), $2k+1$ for $k \leq 7$ due to Butcher (1965b) and Gear (1965). With $\nu = 2$, Butcher (1967) has shown that the hybrid formula (1.18) is stable for $k \leq 15$ with an order $2k+2$. It may be pointed out here that with no off-step point (1.18) can achieve its maximal order satisfying the zero stability condition only for $k < 3$.

1.5 METHODS FOR SOLVING STIFF SYSTEMS

1.5.1 Initial Value Problems for Stiff Systems

Classical methods of Runge-Kutta, Adams etc, are not efficient for the solution of the systems (1.5) if it exhibits the property of 'stiffness'. A single equation may also possesses stiffness. A stiff system is a problem having widely differing time constants or as a system with a large Lipschitz Constant. Generally, stiff systems arise directly or indirectly while modelling many physical problems like chemical kinetics, electronics circuits, control theory, thermal oil recovery, biomathematics, heat conduction, and so on. Mathematically, a stiff system can be defined as follows. [cf. Lambert (1973), Cash (1979)].

Definition 1.7 The linear system of ordinary differential equations

$$\underline{Y}' = \underline{A}\,\underline{Y} + \underline{g}(x), \quad \underline{Y} \in \mathbb{R}^N$$

is said to be stiff if

i) $\mathrm{Re}(\lambda_j) < 0, \quad j = 1,2,\ldots, N$,

and

ii) $\max\limits_{j=1,\ldots,N} |\mathrm{Re}(\lambda_j)| \gg \min\limits_{j=1,\ldots,N} |\mathrm{Re}(\lambda_j)|$,

where, λ_j, $j = 1,2,\ldots, N$ are the eigenvalues of $\underline{A}$.

Definition 1.8 The non-linear system (1.5) is said to be stiff in an interval I of x, if for every $x \in I$,

i) $Re(\lambda_j) < 0, \quad j = 1, \ldots, N$,

ii) $S(x) = \max_{j=1,\ldots,N} |Re(\lambda_j)| / \min_{j=1,\ldots,N} |Re(\lambda_j)| >> 0$,

where, λ_j are the eigenvalues of the Jacobian matrix $\frac{\partial \underline{f}(x, \underline{y}(x))}{\partial \underline{y}}$ evaluated on the solution y(x) at x.

The ratio S(x) can be termed as 'Stiffness ratio' of the problem and generally it ranges from O(10) to $O(10^6)$. A problem is called marginally stiff if S(x) is of O(10) and very stiff if S(x) is of $O(10^6)$. Hence, the stiffness of any system can simply mean that if either of the two ratios, the ratio of largest time constant to the smallest time constant or the ratio of length of time interval of integration to smallest time constant, bears a large, number upto $O(10^6)$.

1.5.2 Implicit Runge-Kutta Methods

A-stability is an essential property of a method to be useful for the solution of stiff systems. In order to have strong stability properties and to provide high accuracy in the solution of stiff systems by Runge-Kutta methods, these methods must be implicit. Implicit Runge-Kutta methods for the stiff systems have first been developed by Butcher (1964b) which is based on Gauss - Legendre quadrature formulas. Butcher (1964b)

has shown that S-stage implicit Runge-Kutta methods can achieve an order of 2S and have the form

$$Y_{n+1} = Y_n + h \sum_{i=1}^{S} b_i F_i , \qquad (1.19a)$$

where, F_i denote the intermediate values computed within the step (x_{n+1}, x_n) and are given by

$$F_i = hf\left(x_n + c_i h,\ Y_n + \sum_{j=1}^{S} a_{i,j} F_j\right) , \qquad (1.19b)$$

$$i = 1,2,\ldots, S.$$

In an array form, Eqn. (1.19) can be written as

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & \cdots & a_{1S} \\ c_2 & a_{21} & a_{22} & \cdots & a_{2S} \\ \vdots & \vdots & \vdots & & \vdots \\ c_S & a_{S1} & a_{S2} & \cdots & a_{SS} \\ \hline & b_1 & b_2 & \cdots & b_S \end{array} = \begin{array}{c|c} c & A \\ \hline & b^T \end{array} ,$$

where $c_i = \sum_{j=1}^{S} a_{ij}$ and $a'_{i,j}s$, $b'_j s$ are constants.

Subsequently, methods based on Gauss-Lobatto quadrature and Gauss - Radau quadrature formulas have been studied by Chipman (1971) and Ehle (1969).

STABILITY properties of Implicit Runge-Kutta Methods : The concept of A-stability can be defined here as [Dahlquist (1963)].

Definition 1.9 The method (1.19) is said to be A-stable if $|y_1| \leq |y_0|$ at any application of it to the linear and autonomous test equation $y' = \lambda y$ with $Re(\lambda) \leq 0$.

Butcher (1975), Burrage and Butcher (1979) and Crouzeix (1979) have introduced the more satisfactory definitions of stability for the implicit Runge-Kutta method (1.19) as B-stability, BN-stability and algebraic stability and are defined as follows:

Definition 1.10 (B-stability) : Let $\ldots y_n, y_{n+1}, \ldots$ and $\ldots z_n, z_{n+1}, \ldots$ be two sequence of approximations of the solution of $y' = f(y(x))$, $f : R^N \longrightarrow R^N$, and $\langle . , . \rangle$ be a scalar product in R^N with $\|.\|$ the corresponding norm. Then the implicit method (1.19) is said to be B-stable iff, for every f satisfying

$$Re \langle f(y) - f(z), y - z \rangle \leq 0, \text{ for all } y, z \in R^N,$$

it holds that

$$\|y_{n+1} - z_{n+1}\| \leq \|y_n - z_n\|.$$

Remark : B-stability implies A-stability.

Definition 1.11 (BN-stability) : If $\{y_n\}$ and $\{z_n\}$ be two sequences of solutions of

$$y'(x) = f(x, y(x)), \quad f : R^{N+1} \longrightarrow R^N$$

with $\langle f(x,y) - f(x,z), y-z \rangle \leq 0, \forall y, z \in R^N$,

then the method (1.19) is said to be BN-stable iff,

$$\|y_{n+1} - z_{n+1}\| \leq \|y_n - z_n\|.$$

Remark : BN-stability implies B-stability.

Definition 1.12 (algebraic stability) : The method (1.19) is said to be algebraic stable iff

i) $b_i \geq 0$, $i = 1,2,\ldots, s$,

and ii) $Q = (q_{ij}) \geq 0$ (non-negative definite),

where, $q_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j$,

$(1 \leq i \leq s,\ 1 \leq j \leq s)$.

It has been seen from the literature that algebraically stable Runge-Kutta methods are more effective than the methods possessing only A-stability.

Definition 1.13 [Dahlquist and Jeltsch (1979)] : The method (1.19) is nonconfluent if all c_i are distinct and confluent otherwise.

The following theorem has been derived by Burrage and Butcher (1979) and Crouzeix (1979).

Theorem 1.3 (i) If the method (1.19) is algebraically stable then it is BN-stable.

(ii) If the method (1.19) is nonconfluent, then conversely, BN-stability implies algebraic stability.

It may be noted here that if one of the b_j in (1.19) is zero, we then have $q_{jj} = 0$ and the non-negative definiteness of Q implies that the jth row of Q must be zero and the method (1.19) becomes reducible [Dahlquist and Jeltsch (1979)]. For an irreducible Runge-Kutta method, the concept of the three stability properties, i.e., B-stability, BN-stability and algebraic

stability are equivalent (Hundsdorfer and Spijiker (1981)). Scherer (1979) has pointed out that Runge-Kutta methods of Lobatto type III_A and III_B (Ehle (1969)) and some other methods do not satisfy the condition of B-stability.

For implementation, fully implicit Runge-Kutta methods suffer from the disadvantage that for each step of integration methods of the type (1.19) require the solution of a system of non-linear algebraic equations of order p(=NxS). However, using a similarity transformation $T^{-1}AT = A1$ where A1 has a much simpler structure, Butcher (1976) has given a very skilful and useful technique for the implementation of general implicit Runge-Kutta methods. Again transforming the Jacobian matrix of the system to Hessenberg form with similarity, rather than using the LU factorization, Varah (1979) has shown that the general Runge-Kutta methods based on Gauss - Legendre, Gauss - Radau and Gauss - Lobatto quadrature formulas can be implemented in a more effective and competitive way. An efficient solution process for the implicit Runge-Kutta methods has also been discussed by Bickart (1977). Algebraically stable Runge-Kutta methods have also been discussed by Hairer (1982), Burrage (1978b).

1.5.3 Semi-explicit Runge-Kutta Methods

It is seen that a set of N-non-linear equations has to be solved for each non-zero diagonal element of the implicit scheme (1.19). In this respect, an enormous gain will be obtained in computational efficiency if for all $i \leq j$, $a_{ij} = 0$

and all the non-zero diagonal elements are equal [Butcher (1976)]. With these properties, the methods (1.19) are called semi-explicit methods and are studied by Norsett (1974) and Alexander (1977). Norsett and Wolfbrandt (1977) have shown that an S-stage semi-explicit Runge-Kutta methods can have maximum order S+1. Deriving some strongly S-stable diagonally implicit Runge-Kutta methods of order 2 in 2-stages and of order 3 in 3-stages. Alexander (1977) has shown that there are no such methods of order four in 4-stages. He has also shown that there is no 4-stage implicit Runge-Kutta methods satisfying A-stability of order five. The necessary and sufficient conditions for A-stability of certain semi-explicit Runge-Kutta methods with one diagonal element of the coefficient matrix equal to zero have been discussed by Cooper and Sayfy (1979). Hairer (1980) has also shown that the highest possible order of an algebraically stable diagonally implicit Runge-Kutta method is four. Other modified Runge-Kutta methods for stiff systems have also been studied by Cash (1975), Van Bokhoven (1980). Considering one method of semi-explicit and another of explicit in pairs, Cooper and Sayfy (1980), 1983) have shown that these methods are also suitable for the integration of stiff systems in an additive fashion to a decomposition of $\underline{f}$ to $\underline{f}_1 + \underline{f}_2$ in (1.5).

1.5.4 Singly - Implicit Runge-Kutta Methods

Singly-implicit Runge-Kutta methods are characterised by a one - point spectrum property of the coefficient matrix and are closely related to the semi-explicit Runge-Kutta methods. These type of methods are first derived by Burrage (1978a) and have been studied in general by Butcher (1981). Stability properties of singly - implicit general linear methods have been studied by Burrage and Chipman (1985).

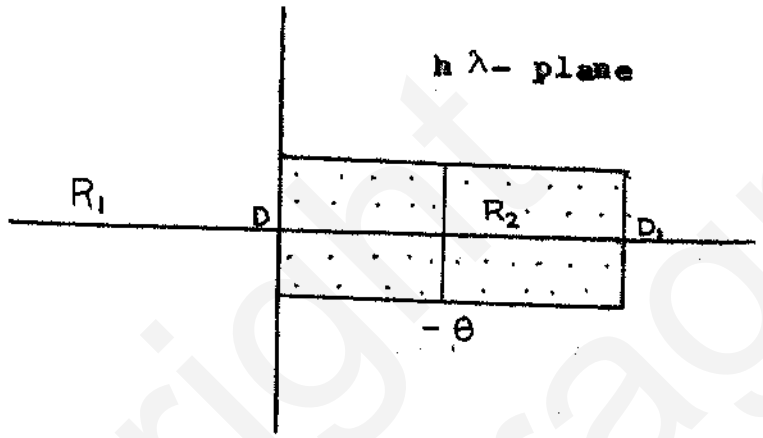
1.5.5 Multistep Methods for Stiff Systems

Multistep methods suitable for the numerical integration of stiff systems should be A-stable and implicit in character. Numerical stability that a multistep method can possess being restricted the accuracy of linear multistep methods suitable for stiff systems is limited. However, greater accuracy can be attained by introducing higher derivatives in the formulas. Second derivative multistep methods for stiff-systems have been discussed by Enright (1972), Liniger and Willoughby (1970), Jackson and Kenue (1974). But the second derivative formulas are not practical for all problems.

In order to achieve linear multistep formulas of an order greater than two, the A-stability requirement should be relaxed. The relaxed stability criterians are those of $A(\alpha)$ - stability due to Widlund (1967) and stiff-stability due to Gear (1969). The following definition is due to Gear (1971).

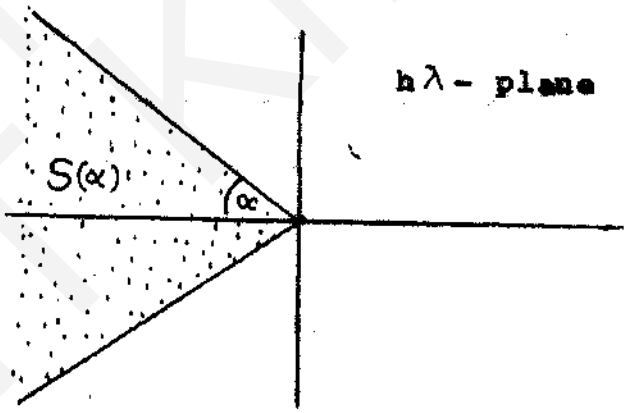
Definition 1.14 A method is stiffly stable if the method when applied to the test equation $y' = \lambda y$, is absolutely stable in R_1 ($Re(h\lambda) \leq D$) and gives accurate solutions in R_2 ($D < Re(h\lambda) < D_1$, $|I_m(h\lambda)| < \Theta$) as shown in Fig.1.1 check

Fig 1.1



A(α)-stability suggested by Widlund (1967) requires that method be absolutely stable in the wedge - region $S(\alpha)$ for any $0 \leq \alpha \leq \pi/2$ as shown in Fig.1.2.

Fig 1.2



Remark : A($\pi/2$)-stable methods are A-stable.

The most successful multistep methods satisfying the above relaxed stability criterian and suitable for stiff ordinary differential equations are the class of backward differentiation formulas (BDF) and are of the form

$$\sum_{j=0}^{k} a_j \, y_{n+1-j} = h \, b_o \, f_{n+1} . \qquad (1.20)$$

Gear (1969, 1971) has shown that these formulas are A(α)-stable and stiffly-stable for $1 \leq k \leq 6$.

We state the following theorems due to Gear (1971).

Theorem 1.4 For multistep methods of order greater than two, no k-step stiffly-stable method can be of order greater than k.

Theorem 1.5 No explicit multistep method can be stiffly-stable.

As the higher order backward differentiation formulas have the poor stability properties, these formulas are not suited to the problems in which the eigenvalues of the Jacobian matrix contain large imaginary parts. Also the performance of the lower order BDF is relatively poor because of their limited accuracy.

Enright et.al (1975) have done a comparing study of various numerical methods on different class of stiff systems. Backward Differentiation Formulas have also been studied by Brayton et.al (1972), stiffly-stable formulas are discussed by Cryer (1972) and Gupta (1976).

NO motivation?

1.6 Motivation and Scope of the Present Study

The present study has been devoted to develop a class of methods which combine the features of both Runge-Kutta and Multistep Methods. These methods rely on some auxiliary points within a step, which have been determined in advance in order to have minimum truncation errors in the formulas. The stability properties of those new methods have been analysed through numerical experiments. It has been seen that these methods are suitable for the integration of both linear and non-linear initial value problems associated with non-stiff and moderately stiff ordinary differential equations of the form (1.1).

In section 1 of chapter II we have developed a class of k-step Auxiliary Explicit Linear Multistep Methods and have shown that these methods are stable with respect to both the errors in the initial values and rounding errors for $k \leq 4$ with one auxiliary point, for $k \leq 5$ with two auxiliary points, for $k \leq 4$ with three auxiliary points, for $k \leq 3$ with four auxiliary points and for $k \leq 2$ with five auxiliary points.

In section 2, we have derived the formulas required to evaluate the dependent variable at the auxiliary points. These auxiliary formulas have been considered without increasing the step number of auxiliary explicit linear multistep methods of section 1 such that each succeeding formula in the entire scheme given for the explicit methods is higher by one.

In section 3, we have derived the auxiliary formulas of the same order as that of the auxiliary explicit linear multistep methods by considering some more previous grid points.

In section 4, in order to have better accuracy, within the existing stability region of a method, the auxiliary formulas are formulated with one more previous grid point, if necessary, than those condidered in the auxiliary formulas of section 3.

The advantages and/or disadvantages of the above various type of formulations of the auxiliary formulas have been discussed in the respective sections of the chapter. The efficiency of the new auxiliary explicit linear multistep methods has also been established by comparing numerical results with some of the existing methods like classical Runge-Kutta methods, Adams-Bashforth- Moulton predictor-corrector methods, Krough's (1966) predictor-corrector method and Schoen's (1971) method of the same order. It has been seen that the new auxiliary linear multistep methods give better accuracy than the methods being compared even with a somewhat larger value of step-length. Having improved stability characteristics, depending on the number of auxliary points used for a particular order, these auxiliary linear multistep methods are competitive for solving moderately stiff systems with a reasonable value of the step-size.

In section 1 of chapter III, a class of k-step Auxiliary Implicit Linear Multistep Methods which are stable with respect to both the errors in the initial values and rounding errors have ?

been developed. These methods satisfy $k \leq 6$ with one auxiliary point, $k \leq 5$ with two auxiliary points, $k \leq 4$ with three auxiliary points, $k \leq 3$ with four auxiliary points and for $k \leq 2$ with five auxiliary points.

In section 2, the auxiliary formulas for the evaluation of the dependent variable at the auxiliary points and the predictor formula have been derived without increasing the step number of the implicit formulas of section 1 such that each succeeding formula in the entire scheme discussed for the auxiliary implicit linear multistep methods in increased by one.

In section 3, by considering some more previous grid points we have derived the auxiliary formulas and predictor formula have been derived of the same order as that of auxiliary implicit linear multistep methods of section 1.

Again considering one more previous grid point in each of the auxiliary formulas and the predictor formula of section 3, new auxiliary formulas and the predictor formula have been derived in section 4, in order to obtain better accuracy within the stability regions.

Some Auxiliary Implicit Linear Multistep Methods which have better stability characteristics than the methods discussed in sections 3 and 4 and which provide better accuracy than the methods of section 2 have been presented in section 5.

The advantages and/or disadvantages of the above different types of auxiliary formulas and predictor formula and the efficiency

of the new implicit schemes over those of Butcher (1965b, 1967), Lonfeld and Thomspn (1967) and other methods being compared in chapter II have been discussed in the respective sections of the chapter. It has been concluded that from a class of k-step methods (where $k \geq 2$) of the same order, it is preferable to choose the method having maximum number of auxiliary points, as it can allow a moderately large value of the step-length h for a desired accuracy in order to save the computational time. It has also been seen from the numerical experiments that the region of stability increases by increasing the number of auxiliary points, order remaining the same.

In contrast to the existing methods for solving stiff equations, the new implicit methods discussed in this chapter are non-iterative and do not require the Jacobian evaluation. Since the stability regions are limited for these new implicit methods compared to that of A-stable methods, they are competitive in solving moderately stiff systems with a reasonable value of the step-size and provide better accuracy.