Computational techniques for the numerical solution of ordinary differential equations

COMPUTATIONAL TECHNIQUES FOR THE NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS

by

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DECLARATION

I declare that the following thesis is a record of research work carried out by me, and that the thesis is of my own composition. I also certify that neither this thesis nor the original work contained therein has been submitted to this or any other institution for a degree.

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CHAPTER 1

INTRODUCTION

1.1 THE EQUATIONS OF MATHEMATICAL PHYSICS

The mathematical formulation of many problems in physics, engineering and economics leads to a relationship between certain unknown quantities (such as distance, pressure, temperature, volume, cost, etc.) and their rate of change with regard to a single independent variable usually representing time, length or angle. This relationship is called an ordinary differential equation. Any of such mathematical formulations can lead to a single differential equation or to a set of differential equations.

The exact solution to an ordinary differential equation in an interval I on the real line is some function which satisfies the differential equation at every point within the interval. For instance, the motion of a body falling freely from rest under the gravitational acceleration g is completely described by the relationship

$$\frac{d^2s}{dt^2} = -g \qquad (1.1.1)$$

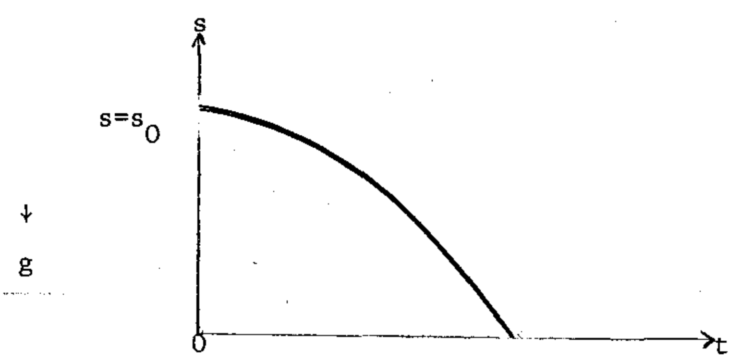

FIGURE (1.1)

The gravitational acceleration acts in the opposite direction to the increasing distance axis as indicated in figure (1.1).

If the initial height of the body is specified as s_0 at time $t=0$, the relationship given by equation (1.1.1) is satisfied at any interval of time $t \geq 0$ by the function $s=s(t)$ given by

$$s(t) = s_0 - \tfrac{1}{2}gt^2 . \tag{1.1.2}$$

For a specified interval I on the real line, it is not always possible to obtain the exact solution to a given ordinary differential equation. For instance, the analytic solution to the Van-der-Pol oscillator:

$$\frac{d^2y}{dx^2} - \varepsilon(1-y^2)\frac{dy}{dx} + y = 0; \quad \varepsilon > 0 \tag{1.1.3}$$

is not known. In an attempt to obtain the numerical solution to such differential equations, there are three basic approaches:

(a) *The Analytic Approximate Method:*

This approach represents the solution to a given differential equation by the sum of a finite number of independent functions. For example, the solution is represented by a truncated power series or the first few terms of an expansion in orthogonal functions or possibly by an asymptotic series, c.f. boundary layer theory in fluid dynamics. These methods are better suited to hand computation but Fox (1962) introduced automatic computation to numerical integration schemes based on Chebyshev polynomials developed by Lanczos (1938) and Clenshaw (1957). Lanczos (1938) based his scheme on polynomial approximations of the form $P_n(x) = \sum_{r=0}^{n} b_r x^r$ and perturbed the right hand side of the differential equation by the term $\tau\, T_n(x)$

to obtain the coefficients of the polynomial, where τ is a real variable and $T_n(x)$ is the Chebyshev polynomial given by

$$T_n(x) = \cos n(\cos^{-1}x) \; ; \; -1 \leq x \leq 1 \; , \tag{1.1.4}$$

Clenshaw (1957) concerned himself with polynomial approximations of the form

$$P_n(x) = \sum_{r=0}^{n} b_r T_r(x) \tag{1.1.5}$$

where $T_r(x)$, $r=0,1,\ldots,n$ are Chebyshev polynomials as given by equation (1.1.4). Fox (1962) demonstrated a close relationship between these two schemes. He also discussed various aspects of these schemes for both initial value and boundary value problems. Details of further work in this area are available in Clenshaw (1962), Lanczos (1957), Fox and Parker (1968), Lyche (1972) and Clenshaw and Norton (1963). This approach is however constrained by the fact that it is only applicable to differential equations whose coefficients are polynomial functions of the independent variable. The scheme is particularly well suited to boundary value problems.

(b) *The Spline Function Approximate Method:*

This approach searches for a global approximate solution to any given initial value problem over the entire interval I of integration (i.e. a continuous solution $z = z(x)$ is sought for in the interval I). The solution is approximated on the interval I by an interpolating polynomial $s_m(x)$ of degree m with the property that $s_m(x)$ possesses continuous derivatives up to and including order m-1. Localzo et.al. (1967) developed schemes for generating the spline approximations to an initial value problem. Blue (1969) established the increased accuracy (although with increased complexity) in the application of spline function approximate method to solving non-linear boundary value problems.

(c) Finite Difference Approximate Methods:

This approach is based on the principle of discretization. Approximate values are sought at a sequence of discrete points on the interval I usually denoted by

$$\{x_i : x_i = x_{i-1} + h,\ i=1,2,\ldots.\} \qquad (1.1.6)$$

if h is the mesh-size. The approach furnishes a set of values $\{y_i\}$ corresponding to the mesh points given by equation (1.1.6). The approximate solution y_i to the exact solution $y(x_i)$ at $x = x_i$ thus contain a discretization error $e_i = y_i - y(x_i)$. Any good algorithm based on discretization will control the discretization errors. This approach has two distinct classes:

(i) One step methods - which only require the solution y_i at $x = x_i$ to obtain the next approximate solution y_{i+1} at $x = x_{i+1}$.

(ii) Multistep methods - which require a certain number of past solutions $y_i, y_{i-1}, y_{i-2} \ldots$ to obtain the approximate solution y_{i+1} at $x = x_{i+1}$.

The finite difference approximate methods are generally well suited to automatic computation and hence are more frequently used and universally applicable.

Localzo and Schoenberg (1967) established a theorem which links the spline function approximate methods to the finite difference approximate methods. For example if the trapezoidal rule, given by

$$y_{t+1} = y_t + \frac{h}{2}(f_t + f_{t+1}),\ t=0,1,\ldots \qquad (1.1.7)$$

[where $\{f_i,\ i=0,1,\ldots\}$ are the values of the derivatives at the mesh points] is repeatedly applied on every sub-interval of I as defined by equation (1.1.6), it is equivalent to approximating the solution y(x) globally on the interval I by a quadratic spline.

We shall adopt the finite difference approximate approach in the development of the new numerical integration algorithms. The other two approaches could also have been adopted except that the constraint on the analytic approximate approach would definitely limit the range of application of the work.

1.2 THE ORDER AND DEGREE OF ORDINARY DIFFERENTIAL EQUATIONS

If the highest derivative that occurs in a differential equation is $\frac{d^n y}{dx^n}$, then the differential equation is said to be of order n. For example, the differential equation (1.1.1) is of order 2. The degree of a differential equation is the power to which the highest derivative is raised, e.g. the differential equation (1.1.1) is of degree 1.

The general form of an ordinary differential equation of order n is given by

$$F(x,y,y^{(1)},\ldots\ldots,y^{(n)}) = 0 \tag{1.2.1}$$

where x is the independent variable, y = y(x) the unknown function and

$$y^{(i)} = \frac{d^i y}{dx^i}, \; i=1,\ldots\ldots,n$$

denotes the i^{th} total derivative of y(x) with respect to x.

Since little can be said about equation (1.2.1), it is assumed that it can be solved locally for the n^{th} derivative of y(x) to give

$$y^{(n)} = G(x,y,y^{(1)},\ldots\ldots,y^{(n-1)}) \tag{1.2.2}$$

The implicit function theorem (Apostol,T.M. 1965) gives the conditions which the function F in equation (1.2.1) must satisfy to be able to obtain equation (1.2.2). Equation (1.2.2) is the normal form for the n^{th} order ordinary differential equation.

We now consider a closed and bounded interval

$$I = a\leq x\leq b \tag{1.2.3}$$

on the real line as our interval of integration. We denote by C^n, a complex n-dimensional space. Let $\underline{\eta} = (\eta_1,\ldots\ldots,\eta_n)$ be a fixed point in C^n and $\underline{f}=(f_1,f_2,\ldots f_n)$, an n-tuple of continuous functions, be a mapping of $R = I \times C^n$ into C^n such that for every $x \in I$ and $\underline{y} = (y_1, \ldots, y_n) \in C^n$

$$\underline{f}(x,\underline{y}) = \underline{y}' = \frac{d\underline{y}}{dx} \in C^n .$$

We shall consider in general, the initial value problem

$$\begin{aligned} \underline{y}' &= f(x,\underline{y}) ; \\ \underline{y}(a) &= \underline{\eta} . \end{aligned} \tag{1.2.4}$$

Equation (1.2.4) constitutes a system of n first order ordinary differential equations. By suitable substitutions, every n^{th} order ordinary differential equations of the form given by equation (1.2.2) can be transformed into a system of n first order ordinary differential equations of the form (1.2.4). For example, the differential equation (1.1.3) which is of second order can be reduced to a system of two first order ordinary differential equations as follows:

$$y_1 = y \quad \text{and} \quad y_1' = y_2 \tag{1.2.5}$$

and substituting these in equations (1.1.3) we obtain

$$y_2' = \varepsilon(1-y_1^2)y_2 - y_1 . \tag{1.2.6}$$

Hence the problem (1.1.3) is transformed to the first order systems:

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= \varepsilon(1-y_1^2)y_2 - y_1 . \end{aligned} \tag{1.2.7}$$

1.3 Vector Norms

As we intend to treat initial value problems in the form given by equation (1.2.4), it is worthwhile to discuss briefly the concept of vector norms. There are many possible vector norms but we shall concern ourselves with the three most commonly applied in practice. A vector norm denoted by $||.||_p$ for $p>0$ is a non-negative function on the space C^n with the following properties:

For arbitrary vectors $\underline{y}$ and $\underline{y}^*$ in C^n and a complex number α,

(a) $||\underline{y}||_p > 0$ if $\underline{y} \neq 0$ (1.3.1)

(b) $||\alpha\underline{y}||_p = |\alpha|.||\underline{y}||_p$ (1.3.2)

(c) $||\underline{y}+\underline{y}^*||_p \leq ||\underline{y}||_p + ||\underline{y}^*||_p$. (1.3.3)

Equation (1.3.3) is known as the triangle inequality.

We now give some examples of the vector norms:

The L_p norm is defined as

$$||\underline{y}||_p = \begin{cases} \left[\sum_{i=1}^{n} |y_i|^p\right]^{\frac{1}{p}} & \text{if } 1 \leq p < \infty \\ \max_{1\leq i\leq n} |y_i| & \text{if } p = \infty \end{cases} \quad . \tag{1.3.4}$$

The most widely used of these norms are:

(i) the sum norm given by

$$||\underline{y}||_1 = \sum_{i=1}^{n} |y_i| , \tag{1.3.5}$$

(ii) the Euclidean norm given by

$$||\underline{y}||_2 = \left(\sum_{i=1}^{n} y_i^2\right)^{\frac{1}{2}} , \tag{1.3.6}$$

and finally,

(iii) the maximum norm given by

$$||\underline{y}||_\infty = \max_{1\leq i\leq n} |y_i| . \tag{1.3.7}$$

In all our applications of vector norms, we shall adopt the maximum norm and denote this as $||.||$. This choice is due to the fact that the maximum norm is more powerful and is comparatively easier to apply than either the sum norm or the Euclidean norm.

1.4 THE EXISTENCE AND UNIQUENESS THEOREM

The integral of an n^{th} order differential equation contains n constants of integration. In other words, this integral constitutes a family of curves in C^n. A particular curve in C^n is only defined if numerical values are attached to the n constants of integration. This is equivalent to specifying the n initial conditions

$$y_i(a) = \eta_i \quad , \; i=1,\ldots,n \tag{1.4.1}$$

for the system (1.2.4).

Before considering conditions for the existence and uniqueness of solutions to an initial value problem, we give the following definition.

The function $\underline{f} = \underline{f}(x,y)$ in equation (1.2.4) is said to satisfy a Lipschitz condition of order one in $\underline{y}$ uniformly in x, if there is a constant L such that the following relation holds,

$$||\underline{f}(x,y) - \underline{f}(x,y^*)|| \leq L||\underline{y} - \underline{y}^*|| \tag{1.4.2}$$

for all $(x,\underline{y})$ and $(x,y^*) \in R$.

We now impose the following constraints on the space C^n:

for every $\quad \underline{y} = (y_1,\ldots,y_n) \in C^n$,

$||\underline{y}|| \leq k_1 < \infty$.

We now state the standard theorem which guarantees the existence of a unique solution to an initial value problem of the form given in equation (1.2.4).

The existence theorem is as follows:

Theorem (1.1)

Let the function $\underline{f} = \underline{f}(x,\underline{y})$ be continuous in the infinite strip $R = I \times C^n$ for all $||\underline{y}|| < \infty$ and satisfy equation (1.4.2). Then, the initial value problem given by equations (1.2.4) has a unique solution $\underline{y} = \underline{y}(x)$ defined on the interval I.

Proof:

If a solution vector $\underline{y}(x)$ actually exists which satisfies the initial condition $\underline{y}(a) = \underline{\eta}$, then from equation (1.2.4), this solution must satisfy the integral equation

$$\underline{y}(x) = \underline{\eta} + \int_a^x f(\alpha, \underline{y}(\alpha))d\alpha \; . \tag{1.4.3}$$

Conversely, if $\underline{y} = \underline{y}(x)$ is continuous and satisfies equation (1.4.3), then it is differentiable and satisfies the equation (1.2.4). The integral equation can now be solved iteratively by Picard's method as follows:

Start with,

$$\underline{y}^{[0]}(x) = \underline{\eta}$$

and then generate the sequence of vector valued functions:

$$\underline{y}^{[r+1]}(x) = \underline{\eta} + \int_a^x \underline{f}(\alpha, \underline{y}^{[r]}(\alpha))d\alpha, \; r=0,1,\ldots \; . \tag{1.4.4}$$

We now wish to show that the sequence of functions $\{\underline{y}^{[r]}(x)\}$ converges absolutely and uniformly to $\underline{y}(x)$ and that the limit function satisfies the integral equation (1.4.3). By taking the norm of the difference of two successive functions generated by equation (1.4.4), we have the following relation:

$$\begin{aligned} ||\underline{y}^{[r+1]} - \underline{y}^{[r]}(x)|| &= ||\left[\underline{\eta} + \int_a^x \underline{f}(\alpha, \underline{y}^{[r]}(\alpha))d\alpha\right] - \\ &\qquad \left[\underline{\eta} + \int_a^x \underline{f}(\alpha, \underline{y}^{[r-1]}(\alpha))d\alpha\right]|| \\ &= ||\int_a^x \left[\underline{f}(\alpha, \underline{y}^{[r]}(\alpha)) - \underline{f}(\alpha, \underline{y}^{[r-1]}(\alpha))\right]d\alpha|| \qquad (1.4.5) \\ &\leq \int_a^x ||\underline{f}(\alpha, \underline{y}^{[r]}(\alpha)) - \underline{f}(\alpha, \underline{y}^{[r-1]}(\alpha))||d\alpha \end{aligned}$$

Since $\underline{f} = \underline{f}(x,y)$ satisfies a Lipschitz condition, we have

$$||\underline{f}(\alpha,\underline{y}^{[r]}(\alpha)) - \underline{f}(\alpha,\underline{y}^{[r-1]}(\alpha))|| \leq L||\underline{y}^{[r]}(\alpha)-\underline{y}^{[r-1]}(\alpha)||. \quad (1.4.6)$$

We now substitute this in equation (1.4.5) to get,

$$||\underline{y}^{[r+1]}(x) - \underline{y}^{[r]}(x)|| \leq L\int_a^x ||\underline{y}^{[r]}(\alpha) - \underline{y}^{[r-1]}(\alpha)||d\alpha. \quad (1.4.7)$$

By similar argument, we have the relation:

$$||\underline{y}^{[r]}(x)-\underline{y}^{[r-1]}(x)|| \leq L\int_a^x ||y^{[r-1]}(\alpha)-\underline{y}^{[r-2]}(\alpha)||d\alpha. \quad (1.4.8)$$

By repeating this procedure (r-2) times, we obtain

$$||\underline{y}^{[3]}(x)-\underline{y}^{[2]}(x)|| \leq L\int_a^x ||\underline{y}^{[2]}(\alpha)-\underline{y}^{[1]}(\alpha)||d\alpha \quad (1.4.9)$$

and finally,

$$||\underline{y}^{[2]}(x)-\underline{y}^{[1]}(x)|| \leq L\int_a^x ||\underline{y}^{[1]}(\alpha)-\underline{y}^{[0]}(\alpha)||d\alpha. \quad (1.4.10)$$

But

$$\begin{aligned} ||\underline{y}^{[1]}(x)-\underline{y}^{[0]}(x)|| &= ||\underline{\eta} + \int_a^x \underline{f}(\alpha,\underline{\eta})d\alpha - \underline{\eta}|| \\ &= ||\int_a^x \underline{f}(\alpha,\underline{\eta})d\alpha|| \\ &\leq \int_a^x ||f(\alpha,\underline{\eta})||d\alpha \end{aligned} \quad (1.4.11)$$

Since the function $\underline{f} = \underline{f}(x,\underline{y})$ is continuous in a closed interval I, then $\underline{f}$ is bounded i.e. there exist a constant $M < \infty$ such that

$$||\underline{f}(x,\underline{y})|| < M \quad (1.4.12)$$

for all $(x,\underline{y}) \in R$.

Using equation (1.4.12) in equation (1.4.11) we obtain,

$$||\underline{y}^{[1]}(x)-\underline{y}^{[0]}(x)|| < M\int_a^x d\alpha = M(x-a) \quad (1.4.13)$$

and this in equation (1.4.10) yields

$$||\underline{y}^{[2]}(x)-\underline{y}^{[1]}(x)|| < LM\int_a^x (\alpha-a)d\alpha = ML\frac{(x-a)^2}{2!}. \quad (1.4.14)$$

Similarly, using equation (1.4.14) in equation (1.4.9) gives

$$\begin{aligned} ||\underline{y}^{[3]}(x)-\underline{y}^{[2]}(x)|| &< \frac{ML^2}{2!}\int_a^x (\alpha-a)^2 d\alpha \\ &= \frac{ML^2}{3!}(x-a)^3 \end{aligned} \quad (1.4.15)$$

By continuing with this procedure, equation (1.4.7) gives the result

$$||\underline{y}^{[r+1]}(x)-\underline{y}^{[r]}(x)|| < \frac{ML^r}{(r+1)!}(x-a)^{r+1} . \qquad (1.4.16)$$

The function $\underline{y}^{[r+1]}(x)$ can be expressed as

$$\underline{y}^{[r+1]}(x) = \underline{y}^{[0]} + \sum_{s=0}^{r} [\underline{y}^{[s+1]}(x)-\underline{y}^{[s]}(x)] . \qquad (1.4.17)$$

By applying equations (1.4.4) and (1.4.16) in equation (1.4.17) we have

$$\|\underline{y}^{[r+1]}(x)\| \leq \|\underline{\eta}\| + \sum_{s=0}^{r} \frac{ML^s}{(s+1)!}(x-a)^{s+1} . \qquad (1.4.18)$$

Now the series

$$\sum_{s=0}^{r} \frac{M}{L} \cdot \frac{[L(x-a)]^{s+1}}{(s+1)!} \qquad (1.4.19)$$

is absolutely and uniformly convergent. Hence the sequence of continuous functions $\{\underline{y}^{[r]}(x)\}$ converges uniformly to $\underline{y}(x)$ on the interval I and the limiting function $\underline{y}(x)$ is necessarily continuous. The limiting function $\underline{y}(x)$ is given by

$$\begin{aligned}\underline{y}(x) = \lim_{r\to\infty} \underline{y}^{[r]}(x) &= \underline{\eta} + \lim_{r\to\infty}\int_a^x \underline{f}(\alpha,\underline{y}^{[r-1]}(\alpha))d\alpha \\ &= \underline{\eta} + \int_a^x \lim_{r\to\infty} \underline{f}(\alpha,\underline{y}^{[r-1]}(\alpha))d\alpha \\ &= \underline{\eta} + \int_a^x \underline{f}(\alpha,\underline{y}(\alpha))d\alpha . \end{aligned} \qquad (1.4.20)$$

Equation (1.4.20) implies that the limiting function $\underline{y}(x)$ satisfies the integral equation and hence the differential equation (1.2.4) for any arbitrary $\underline{\eta} \in C^n$.

Next we discuss the uniqueness of the solution.

Suppose there is another solution $\underline{z}(x)$ to the initial value problem (1.2.4) with $\underline{z}(a) = \underline{\eta}$. $\underline{z}(x)$ must satisfy the integral equation (1.4.3). Hence

$$\underline{z}(x) = \underline{\eta} + \int_a^x \underline{f}(\alpha,\underline{z}(\alpha))d\alpha. \qquad (1.4.21)$$

By subtracting equation (1.4.4) from equation (1.4.21) and taking norms, we obtain

$$||\underline{z}(x)-\underline{y}^{[r+1]}(x)|| = ||\int_a^x \underline{f}(\alpha,\underline{z}(\alpha))d\alpha - \int_a^x \underline{f}(\alpha,\underline{y}^{[r]}(\alpha))d\alpha||$$

$$\leq \int_a^x ||\underline{z}(\alpha)-\underline{y}^{[r]}(\alpha)||d\alpha \quad . \qquad (1.4.22)$$

For r=0, equation (1.4.22) gives

$$||\underline{z}(x)-\underline{y}^{[1]}(x)|| \leq L\int_a^x ||z(\alpha)-\underline{\eta}||d\alpha \quad . \qquad (1.4.23)$$

But

$$||\underline{z}(x)-\underline{\eta}|| = ||\underline{z}(x) + (-\underline{\eta})|| \leq ||\underline{z}(x)||+||\underline{\eta}||$$

$$\leq k_1+k_1 = k_2 \text{ say} \quad . \qquad (1.4.24)$$

Hence, equation (1.4.23) implies

$$||\underline{z}(x)-\underline{y}^{[1]}(x)|| \leq Lk_2(x-a)$$

For r=2, we have

$$||\underline{z}(x)-\underline{y}^{[2]}(x)|| \leq k_2 \frac{L^2(x-a)^2}{2!}$$

and in general, we have

$$||\underline{z}(x)-y^{[s]}(x)|| \leq k_2 \frac{[L(x-a)]^s}{s!} \quad . \qquad (1.4.25)$$

Hence

$$\lim_{s\to\infty} ||\underline{z}(x)-\underline{y}^{[s]}(x)|| = 0 \quad . \qquad (1.4.26)$$

Therefore,

$$\underline{z}(x) = \lim_{s\to\infty} \underline{y}^{[s]}(x) = \underline{y}(x) \quad .$$

Hence, the limiting function y(x) is the unique solution to the initial value problem (1.2.4).

It is very essential to ascertain the existence of solutions to an initial value problem before we embark on obtaining its numerical solution. Some numerical integration schemes will still give results although meaningless even though the initial value problem has no solution or it has a solution but it is not unique. For instance, the initial value problem

$$y' = -\sqrt{1-y^2} \quad ; \; y(0) = 1$$

does not satisfy the Lipschitz condition in y at x = 0 since

$$\left.\frac{\partial f}{\partial y}\right|_{x=0} = \left.\frac{y}{\sqrt{1-y^2}}\right|_{x=0} = \infty$$

although $|f(x,y)| \leq 1 \;\; \forall\, x$.

In fact, the family of solutions is

$$y = \cos(x+\alpha) \;,\; \alpha \text{ real };$$

y = +1 is thus a solution of a special kind.

If this problem is solved with any numerical integration scheme which does not make use of higher derivatives of f(x,y) the values returned will be y = +1 for all values of x.

In passing, we remark that any desired accuracy in the numerical integration of an initial value problem can be attained (if the problem satisfies a Lipschitz condition with respect to the dependent variable) by choosing a sufficiently small mesh size. However, the effect of rounding off errors is magnified owing to the larger computation involved with decreasing mesh size.

1.5 Some Examples

We now discuss briefly some physical problems which lead to ordinary differential equations containing discontinuities as well as those ordinary differential equations whose solutions are periodic.

The problem (1.1.1) can be considered as a practical example of a system of ordinary differential equations with discontinuous derivatives if the objects dropped were inelastic. The motion is completely destroyed at the point of impact with the ground.

Examples of systems of ordinary differential equations having oscillatory (in particular, periodic) solutions are of considerable interest in stability theory in control. Notable amongst these equations are the celebrated problems of the Van-der-Pol oscillator and the Rayleigh's oscillator.

a) *The Van-der-Pol Oscillator*

The Van-der-Pol oscillator with control is given by the equation

$$y''-\mu(1-y^2)y' + ay + k = 0 \tag{1.5.1}$$

where μ,k and a are positive real numbers and k is the control parameter. The system (1.5.1) has attracted much attention in control theory since it was first discussed by B. Van-der-Pol in 1926. The attraction is perhaps due to the curious nature of its phase portraits which provide an excellent example of the limit cycle approached both from within and without by the phase trajectories. The phase portrait of the problem (1.5.1) for $\mu = +2$, and control $k = -0.5$ has been obtained by Fatunla (1972) (see figure 1.2).

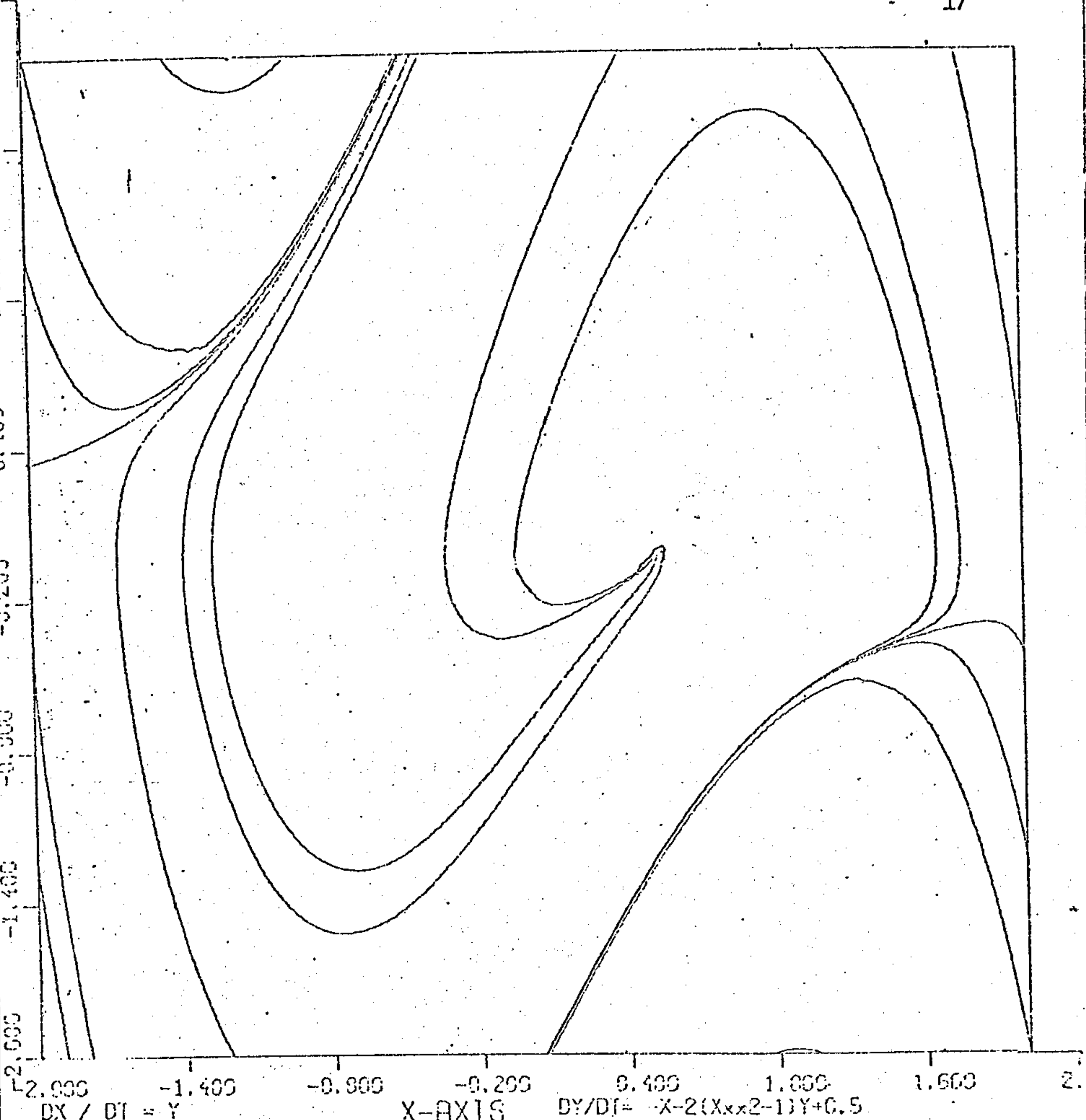
-2.000
-1.400
-0.800
-0.200
0.400
1.000
1.600
2.
DX / DT = Y
X-AXIS
DY/DT= -X-2(X**2-1)Y+0.5

FIGURE 1.2

The problem (1.5.1) is solved with the new schemes to be given later for the case $\mu = 0.01$, $a = 1$ and $k = 0$.

Rayleigh's Equation

The Rayleigh's oscillator is given by the differential equation:

$$y'' + ky' + n^2 y = 0 \,. \tag{1.5.2}$$

Lord Rayleigh (1894) in his 'Theory of Sound' argued that the problem (1.5.2) defines a steady vibration if $k = 0$ and that if k is positive, the vibration will die down and if k is negative, the vibration will increase without limit. This problem is solved for $k = 0$, $n = 1$ with all the new numerical integration procedures given in Chapters IV, V and VI.

1.6 THE EXISTING NUMERICAL INTEGRATION SCHEMES

As the main objective of this text is to develop some new integration algorithms for solving initial value problems in ordinary differential equations containing discontinuities as well as those whose solutions are oscillatory, we shall give a brief account of past activities in these areas.

Amongst the existing schemes is one by Goran Fick (1971) which is a modification of the IBM subroutine named DHAMDI and is based on Hamming's predictor corrector scheme. The scheme identifies the point of discontinuity if the mesh size has been halved a certain number of times and the numerical solution does not meet the tolerance requirement. Another scheme to solve discontinuous systems was developed by O'Regan (1970). His Alpha scheme is based on the fourth order Runge-Kutta integration scheme whilst a detector function is introduced which identifies the point of discontinuity when there is a change in the sign of the detector function. This procedure makes use of Newton-Raphson's iteration scheme to solve a non-linear equation for the fraction of the current stepsize to determine the point of discontinuity. The resultant scheme yields a third order Runge-Kutta algorithm. The latest effort in this area includes the work of Hay et.al (1974) who used a sequence of detector functions to locate the points of discontinuity. The point of discontinuity is identified with the change in the sign of one of the detector functions.

Gautschi (1961) developed a multistep scheme for solving ordinary differential equations having periodic solutions. His integration algorithm is based on annihilating trigonometric polynomials up to a desired degree. As the coefficients of the resultant multistep schemes are functions of the period of the solution, an a priori knowledge of the period is essential.

1.7 PREVIEW

In the subsequent chapters, new explicit one-step and linear multi-step numerical integration schemes are proposed with the view of obtaining maximum stability characteristics.

Chapter II gives a brief background of some numerical methods that are relevant to the development of the new integration schemes proposed in subsequent chapters. A brief account of Gautschi's integration scheme as well as Lambert and Shaw's integration schemes is also given.

Chapter III deals exclusively with the adaptation of the Gragg, Bulirsch and Stoer algorithm to solve initial value problems containing discontinuities.

In Chapter IV, we propose a new variable order one step integration scheme. The scheme is based on representing the solution in every sub-interval by the combination of a polynomial and trigonometric or hyperbolic interpolant. The convergence and stability of the scheme are also established.

In Chapter V, an explicit linear multistep scheme is developed. It is based on the same set of interpolants as in Chapter IV.

Finally, in Chapter VI we develop a linear multistep scheme to integrate special second order systems. A brief comparison of the new schemes proposed in Chapters IV, V and VI with some of the existing schemes is presented.

CHAPTER II

BACKGROUND NUMERICAL ANALYSIS

2.1 INTRODUCTION

In this chapter, we shall discuss briefly some of the basic numerical analysis which is relevant to the development of the new integration algorithms in the subsequent chapters. The discussion includes:

(a) difference operators

(b) finite difference approximate methods for solving initial value problems in ordinary differential equations

(c) some finite difference methods for solving special problems in ordinary differential equations namely

(i) Gautschi's multistep methods for solving initial value problems having periodic or oscillatory solutions, and

(ii) Lambert and Shaw's algorithm for solving initial value problems whose solutions contain singularities.

2.2 THE DIFFERENCE OPERATORS

Let $\{x_t, t=0,1,...\}$ be the mesh points on the interval I defined by the equation (1.1.6). Suppose the values $\{y_t: y_t=y(x_t)$ $t=0,1,...\}$ of the function $y=y(x)$ are known at these mesh points.

We first introduce the shift operator denoted by E and defined by

$$E^k y_t = y_{t+k}, \qquad t=0,1,.... \tag{2.2.1}$$

where k is a real number.

We now define the following difference operators:

(a) the forward difference operator denoted by Δ and defined by

$$\begin{aligned}\Delta y_t &= y_{t+1} - y_t \\ &= E^1 y_t - E^0 y_t \\ &= (E-1)y_t \end{aligned} \quad (2.2.2)$$

(b) the backward difference operator denoted by ∇ and defined by

$$\begin{aligned}\nabla y_t &= y_t - y_{t-1} \\ &= E^0 y_t - E^{-1} y_t \\ &= (1-E^{-1})y_t \end{aligned} \quad (2.2.3)$$

(c) the central difference operator denoted by δ and defined by

$$\begin{aligned}\delta y_t &= y_{t+\frac{1}{2}} - y_{t-\frac{1}{2}} \\ &= E^{\frac{1}{2}} y_t - E^{-\frac{1}{2}} y_t \\ &= (E^{\frac{1}{2}}-E^{-\frac{1}{2}})y_t \,. \end{aligned} \quad (2.2.4)$$

These operators satisfy the commutative, associative and distributive laws.

The higher order forward differences can be obtained as follows:

$$\begin{aligned}\Delta^p y_t &= (E-1)^p y_t \\ &= \sum_{r=0}^{p} (-1)^r \binom{p}{r} E^{p-r} y_t \\ &= \sum_{r=0}^{p} (-1)^r \binom{p}{r} y_{t+p-r} \end{aligned} \quad (2.2.5)$$

Similar expressions can be obtained for the backward and central differences.

We end this section with the statement of the following theorem whose proof is available in Young and Gregory (1973).

Theorem 2.1

If f(x) is a polynomial of degree <n, then

(i) $\Delta^n f(x) = 0$,

(ii) $\nabla^n f(x) = 0$,

(iii) $\delta^n f(x) = 0$.

2.3 One-Step Methods for Solving Ordinary Differential Equations

A general one-step scheme for obtaining the numerical solution of the initial value problem (1.2.4) can be written in the form:

$$\underline{y}_0 = \underline{\eta} ,$$

$$\underline{y}_{t+1} = \underline{y}_t + h\underline{\phi}(x_t,\underline{y}_t;h), t=0,1,\ldots \qquad (2.3.1)$$

where the increment function $\underline{\phi} = \underline{\phi}(x,\underline{y};h)$ is determined by the function $\underline{f} = \underline{f}(x,\underline{y})$ and is a function of $x_t,\underline{y}_t$ and h only.

We now give the following definitions:

Definition (2.3.1)

If p is the largest integer for which the difference between the numerical solution $\underline{y}_{t+1}$ at $x=x_{t+1}$ given by equation (2.3.1) and the theoretical solution $\underline{y}(x_{t+1})$ satisfies the following relationship:

$$\underline{y}_{t+1} - \underline{y}(x_{t+1}) = 0(h^{p+1}), \qquad (2.3.2)$$

then the one-step scheme given by equation (2.3.1) is said to be of order p.

Definition (2.3.2)

The one-step scheme defined by equation (2.3.1) is said to be consistent with the initial value problem (1.2.4) if the increment function satisfies the following relation:

$$\underline{\phi}(x_t, \underline{y}_t; 0) \equiv \underline{f}(x_t, \underline{y}_t) \quad . \qquad (2.3.3)$$

Definition (2.3.3)

The one step scheme defined by equation (2.3.1) is said to be convergent for arbitrary initial value $\underline{\eta}$ and arbitrary $x \in I$ if,

$$\lim_{\substack{h \to 0 \\ x_t \to x}} \underline{y}_t = \underline{y}(x) \quad . \qquad (2.3.4)$$

Henrici (1962) proved that if the increment function $\underline{\phi} = \underline{\phi}(x, \underline{y}; h)$ is continuous in the interval I with respect to $x, \underline{y}$ and h; and if it satisfies a Lipschitz condition with respect to $\underline{y}$ in the region R, then the one step scheme (2.3.1) is convergent if and only if it is consistent.

Definition (2.3.4)

A one step scheme is said to be stable if for each differential equation satisfying a Lipschitz condition, there exists positive constants h_0 and k such that the difference between two different numerical solutions $\underline{y}$ and $\underline{y}^*$ each satisfying equation (2.3.1) is such that

$$||\underline{y}_t - \underline{y}_t^*|| \leq k||\underline{\eta} - \underline{\eta}^*|| \qquad (2.3.5)$$

for all $0 \leq h \leq h_0$, where

$$\underline{y}(a) = \underline{\eta}$$

and $$\underline{y}^*(a) = \underline{\eta}^* .$$

2.4 Explicit Linear Multistep Methods For Integrating Systems of Ordinary Differential Equations

A general linear explicit multistep scheme of step number k can be written in the form:

$$\sum_{j=0}^{k} \alpha_j y_{t+j} = h \sum_{j=0}^{k} \beta_j f_{t+j} \qquad (2.4.1)$$

where $f_{t+j} = f(x_{t+j}, y_{t+j})$; and $\{\alpha_j, \beta_j;\ j=0,1,\ldots k\}$ denote real constants with the following constraints,

$$\alpha_k \neq 0, \ \beta_k = 0 \text{ and } |\alpha_0| + |\beta_0| > 0.$$

Definition (2.4.1)

The linear multistep scheme given by equation (2.4.1) is said to be convergent for all initial value problems subject to the hypothesis of theorem (1.1), if the relation

$$\lim_{\substack{h\to 0\\ th=x-a}} y_t = y(x_t) \qquad (2.4.2)$$

holds for all $x \in I$ and for all solutions $\{y_t\}$ of the difference equation (2.4.1) satisfying the starting conditions

$$y_\mu = \eta_\mu(h) \qquad (2.4.3)$$

for which

$$\lim_{h\to 0} \eta_\mu(h) = \eta \ , \qquad (2.4.4)$$

$$\mu = 0,1,\ldots,k-1.$$

With the view of defining the order of the linear multistep scheme of the form given by equation (2.4.1), we as in Henrici (1962), associate with equation (2.4.1) a linear difference operator given by

$$\mathcal{L}\left[y(x); h\right] = \sum_{j=0}^{k} \left[\alpha_j y(x+jh) - h\beta_j y'(x+jh)\right] \qquad (2.4.5)$$

for an arbitrary function $y(x)\epsilon C^{\infty}[a,b]$.

The Taylor's series expansion of $y(x+jh)$ at x gives

$$y(x+jh) = y(x) + \sum_{i=1}^{\infty} \frac{(jh)^i}{i!} y^{(i)}(x) \tag{2.4.6}$$

and the Taylor's series expansion of $y'(x+jh)$ at x gives

$$y'(x+jh) = y'(x) + \sum_{i=1}^{\infty} \frac{(jh)^i}{i!} y^{(i+1)}(x) \quad . \tag{2.4.7}$$

Using equations (2.4.6) and (2.4.7) in equation (2.4.5) and collecting terms, we obtain

$$\mathcal{L}[y(x);h] = \sum_{i=0}^{\infty} c_i h^i y^{(i)} \tag{2.4.8}$$

where c_i, $i=0,1,\ldots$ are constants.

Definition (2.4.2)

The difference operator $\mathcal{L}$ defined by equation (2.4.8) and the associated linear multistep scheme given by equation (2.4.1) are said to be of order p if

$$c_i = 0 \quad i \leq p$$

and $c_{p+1} \neq 0$

The constants c_i, $i=0,1,2,\ldots$ in equation (2.4.8) are given as follows:

$$c_0 = \sum_{i=0}^{k} \alpha_i$$

$$c_1 = \sum_{i=0}^{k} i\alpha_i - \sum_{i=0}^{k} \beta_i \tag{2.4.9}$$

and

$$c_r = \frac{1}{r!} \cdot \sum_{i=0}^{k} i^r \alpha_i - \frac{1}{(r-1)!} \sum_{i=0}^{k} i^{r-1} \beta_i, \quad r=2,3,\ldots \quad .$$

The parameters $\{\alpha_j, \beta_j;\ j=0,1,\ldots,k\}$ can be obtained from equation (2.4.9). The local truncation error at $x=x_{t+k}$ for an explicit linear multistep scheme is simply the difference between the theoretical solution given by $y(x_{t+k})$ and the numerical solution y_{t+k} obtained by (2.4.1). The definition makes the simplifying assumption that there were no previous errors i.e. $y_{t+j} = y(x_{t+j})$, $j=0,1,\dots,k-1$.

Definition (2.4.3)

The linear multistep method given by equation (2.4.1) is said to be consistent if it has order $p \geq 1$ i.e. that the first two constants c_0 and c_1 in equation (2.4.9) should vanish. This implies

$$\sum_{j=0}^{k} \alpha_j = 0 \tag{2.4.10}$$

and

$$\sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_j . \tag{2.4.11}$$

The first characteristic polynomial $\rho(s)$ of (2.4.1) is defined by

$$\rho(s) = \sum_{j=0}^{k} \alpha_j s^j \tag{2.4.12}$$

and the second characteristic polynomial $\sigma(s)$ is given by

$$\sigma(s) = \sum_{j=0}^{k} \beta_j s^j . \tag{2.4.13}$$

From equations (2.4.10) to (2.4.13), we can deduce that the multistep scheme given by equation (2.4.1) is consistent if and only if the characteristic polynomials satisfy the following conditions

$$\rho(1) = 0$$

$$\rho'(1) = \sigma(1) . \tag{2.4.14}$$

Definition (2.4.4)

The linear multistep scheme given by equation (2.4.1) is said to be zero-stable if no root of the first characteristic polynomial has modulus greater than unity and that every root of unit modulus is simple.

Henrici (1962) established that the necessary and sufficient conditions for the linear multistep scheme given by equation (2.4.1) to be convergent is that it be consistent and zero-stable.

2.5 MULTISTEP SCHEMES FOR PERIODIC OR OSCILLATORY SYSTEMS. (GAUTSCHI 1961)

Gautschi (1961) formulated a non-linear multistep scheme for solving initial value problems whose solutions are periodic or oscillatory with known periods. The scheme integrates exactly appropriate trigonometric polynomials of given orders in precisely the same manner that the classical methods integrate exactly algebraic polynomials of given orders.

If the known or estimated period of the solution to an initial value problem is T, the frequency is then given by

$$\omega = \frac{2\pi}{T} .$$

Gautschi's multistep method is then defined by

$$\sum_{j=0}^{k} \alpha_j y_{t+j} = h \cdot \sum_{j=0}^{k} \beta_j(v)\, f_{t+j} \tag{2.5.1}$$

where $\alpha_k = +1$ and $v = \omega h$. (2.5.2)

Definition (2.5.1)

The multistep scheme given by equations (2.5.1) and (2.5.2) is said to be of trigonometric order r relative to the frequency ω if the associated linear difference operator $\mathcal{L}_\omega$ defined by the relationship;

$$\mathcal{L}_{\omega}[y(x);h] = \sum_{j=0}^{k}[\alpha_j y(x+jh)-h\beta_j(v)y'(x+jh)] \tag{2.5.2}$$

for an arbitrary $y(x) \varepsilon C^{\infty}[a,b]$
satisfies the following conditions:

$$\text{(a)}\mathcal{L}_{\omega}[1;h] \equiv 0, \tag{2.5.3}$$

$$\text{(b)}\mathcal{L}_{\omega}[\cos(s\omega x);h] \equiv \mathcal{L}_{\omega}[\sin(s\omega x);h] \equiv 0, \quad s=1,2,\ldots,r \tag{2.5.4}$$

$$\text{(c)}\mathcal{L}_{\omega}[\cos((r+1)\omega x);h] \quad \text{and} \quad \mathcal{L}_{\omega}[\sin((r+1)\omega x);h] \tag{2.5.5}$$

are not both identically zero.

The trigonometric order r of a multistep scheme is less than the algebraic order p as equation (2.5.4) requires two conditions for each $s \geq 1$ instead of the one condition in equation (2.4.9).

Gautschi proved the following result on the trigonometric order attainable by the multistep scheme given by equation (2.5.1) with a given step number k. He showed that for any given set of coefficients $\{\alpha_j, \ j=0,1,\ldots,k\}$ satisfying the relation

$$\sum_{j=0}^{k} \alpha_j = 0, \tag{2.5.6}$$

there exists a unique explicit method of class (2.5.1) whose trigonometric order $r=\frac{1}{2}k$ and that if the frequency ω vanishes, then the scheme (2.5.1) reduces to a linear multistep scheme with algebraic order $p=2r$.

The Adams' type method with step number k=2 is given as follows:

$$y_{t+2} = y_{t+1} + h[\beta_0(v)f_t + \beta_1(v)f_{t+1}], \tag{2.5.7}$$

where

$$\beta_0(v) = -\frac{1}{2}(1+\frac{1}{12}v^2 + \frac{1}{120}v^4 + \ldots\ldots), \tag{2.5.8}$$

and

$$\beta_1(v) = \frac{3}{2}\left(1 - \frac{1}{4}v^2 + \frac{1}{120}v^4 + \ldots\ldots\right). \qquad (2.5.9)$$

Equations (2.5.7) to (2.5.9) yield a multistep scheme of trigonometric order r=1 and algebraic order p=2.

If the step number k=4, the multistep integration formula is given by:

$$y_{t+4} = y_{t+3} + h\left[\beta_0(v)f_t + \beta_1(v)f_{t+1} + \beta_2(v)f_{t+2} + \beta_3(v)f_{t+3}\right], \qquad (2.5.10)$$

with coefficients given by

$$\beta_0(v) = -\frac{9}{24}\left(1 + \frac{1}{4}v^2 + \frac{11}{120}v^4 + \ldots\right), \qquad (2.5.11)$$

$$\beta_1(v) = \frac{37}{24}\left(1 - \frac{421}{444}v^2 + \frac{1921}{13320}v^4 + \ldots\right), \qquad (2.5.12)$$

$$\beta_2(v) = -\frac{59}{24}\left(1 - \frac{923}{708}v^2 + \frac{15647}{21240}v^4 + \ldots\right), \qquad (2.5.13)$$

and

$$\beta_3(v) = \frac{55}{24}\left(1 - \frac{95}{132}v^2 + \frac{79}{792}v^4 + \ldots\right). \qquad (2.5.14)$$

Equations (2.5.10) to (2.5.14) yield a multistep scheme of trigonometric order r=2 and algebraic order p=4.

2.6 SPECIAL METHODS FOR SOLVING INITIAL VALUE PROBLEMS WHOSE SOLUTIONS POSSESS SINGULARITIES

Lambert and Shaw (1965, 1966) developed both the one-step and multistep schemes which are based on local non-polynomial interpolating functions. They suggested the local interpolant;

$$F(x) = \begin{cases} \sum_{i=0}^{L} a_i x^i + \beta|A+x|^M, \text{ if } M \notin \{0,1,\ldots,L\} \\ \sum_{i=0}^{L} a_i x^i + \beta|A+x|^M \log|A+x| \text{ if } M \in \{0,1,\ldots,L\} \end{cases} \quad (2.6.1)$$

where L is a positive integer, β and $\{a_i, i=0,1,\ldots,L\}$ are real undetermined coefficients; M and A are real parameters which control the nature and position of the singularities.

The L+2 undetermined coefficients are eliminated by imposing the following constraints on the interpolant (2.6.1):

$$y_t = F(x_t) \ , \quad (2.6.2)$$

$$y_{t+1} = F(x_{t+1}),$$

and $$y_t^{(i)} = F^{(i)}(x_t), \ i=1,\ldots,L+1 \ .$$

The resultant integration formulae are given as follows:

$$y_{t+1} = y_t + \sum_{i=1}^{L} \frac{h^i}{i!} y_t^{(i)} + \frac{(A_{(t)}+x_t)^{L+1}}{\alpha^M_{L}(t)} y_t^{(L+1)}$$

$$\times \left[\left[1+ \frac{h}{A_{(t)}+x_t}\right]^{M(t)} - 1 - \sum_{i=1}^{L} \frac{\alpha^{M(t)}_{i-1}}{i!} \left[\frac{h}{A_{(t)}+x_t}\right]^i \right]$$

$$M_{(t)} \notin \{0,1,\ldots,L\}, \quad (2.6.3)$$

and

$$y_{t+1} = y_t + \sum_{i=1}^{L} \frac{h^i}{i!} y_t^{(i)} + \frac{(-1)^{L-M(t)} (A_{(t)}+x_t)^{L+1} y_t^{(L+1)}}{M_{(t)}!(L-M_{(t)})!} \times$$

$$\left[\left(1+ \frac{h}{A_{(t)}+x_t}\right)^{M(t)} \log\left(1+ \frac{h}{A_{(t)}+x_t}\right) - \sum_{i=1}^{L} \left\{ \frac{h^i \alpha^{M(t)}_{i-1}}{i!(A_{(t)}+x_t)^i} \sum_{j=0}^{i-1} \frac{1}{M_{(t)}-j} \right\} \right],$$

$$M_{(t)} \in \{0,1,\ldots,L\} \quad (2.6.4)$$

where

$$\alpha_r^m = m(m-1).....(m-r), \tag{2.6.5}$$

for a non-negative integer r and the parameters $M_{(t)}$, $A_{(t)}$ are given by

$$M_{(t)} = L+1+ \frac{(y_t^{(L+2)})^2}{(y_t^{(L+2)})^2 - y_t^{(L+1)}\, y_t^{(L+3)}}, \tag{2.6.6}$$

and

$$A_{(t)} = -x_t + \frac{y_t^{(L+2)}\, y_t^{(L+1)}}{(y_t^{(L+2)})^2 - y_t^{(L+1)}\, y_t^{(L+3)}}. \tag{2.6.7}$$

$M_{(t)}$ and $A_{(t)}$ are the estimates of the parameters M and A at $x = x_t$.

Both the one-step integration formulae given by equations (2.6.3) and (2.6.4) are of order L+1 and the local truncation error is given by

$$T_{t+1} = \sum_{s=L+2}^{\infty} \frac{h^s}{s!} \left[y_t^{(s)} - \frac{\alpha_{s-L-2}^{M_{(t)}-L-1}\, y_t^{(L+1)}}{(A_{(t)}+x_t)^{s-L-1}} \right], \tag{2.6.8}$$

with $\alpha_s^{M(t)}$ given by equation (2.6.5).

We shall use a similar approach as in this section to develop new integration formulae for solving initial value problems in ordinary differential equations whose solutions are oscillatory. The new integration formulae will be compared with the integration procedure discussed in section (2.5).

CHAPTER III

A RATIONAL EXTRAPOLATION SCHEME FOR INTEGRATING SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS CONTAINING DISCONTINUITIES

3.1 INTRODUCTION

In this Chapter, an adaptation of the work of Bulirsch and Stoer (1966) together with Gragg's modified midpoint scheme (1964) is presented for the integration of systems of ordinary differential equations containing discontinuities. Certain detector functions are introduced and the points of discontinuity are defined as the intersection of the solution to the initial value problem with the zeros of the given algebraic equations. Since the detector functions in general have not only the independent variable as argument but also the solution vector of the initial value problem, it is desirable to determine the solution to the initial value problem very accurately. The rational extrapolation scheme has distinguished itself amongst the best of numerical integration schemes for solving initial value problems in ordinary differential equations (Hull et al., 1972) It is therefore not out of place to adapt the same scheme to integrate systems of ordinary differential equations having discontinuous derivatives. Certain properties of the extrapolation procedure are exploited to accelerate the accurate determination of the points of discontinuity.

3.2 FORMULATION OF THE PROBLEM

We consider the initial value problem,

$$\frac{d\underline{y}}{dx} = \underline{f}(x,\underline{y}) \quad , \quad (x,\underline{y}) \in R \tag{3.2.1}$$

$$\underline{y}(a) = \underline{\eta}$$

and the discontinuity condition is given by,

$$\gamma(x,\underline{y}) = 0. \tag{3.2.2}$$

We now make the simplifying assumption that each component $f_i = f_i(x,\underline{y})$ of $\underline{f}$ given by equation (3.2.1) is at least piecewise continuous in x within the chosen interval I.

It is desired to determine the intersection of the solution vector of problem (3.2.1) with the zeros of the function $\gamma = \gamma(x,\underline{y})$ defined by equation (3.2.2) in the region R.

An integer N is chosen to obtain a uniform mesh-size,

$$h = \frac{b-a}{N}. \tag{3.2.3}$$

With this mesh-size, the interval I is subdivided as

$$I = \bigcup_{r=0}^{N-1} I_r, \tag{3.2.4}$$

where each subinterval I_r is given by

$$I_r := x_r \leq x \leq x_{r+1} = x_r + h, \; r=0,1,\ldots,N-1. \tag{3.2.5}$$

Hence, the relation

$$I_r \cap I_{r+1} = x_{r+1}, \; r=0,1,\ldots,N-1 \tag{3.2.6}$$

holds.

In the next section, we shall develop the Gragg-Bulirsch-Stoer algorithm for solving systems of ordinary differential equations of the form (3.2.1).

3.3 THE GRAGG-BULIRSCH-STOER ALGORITHM FOR SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS

We shall apply the Gragg-Bulirsch-Stoer algorithm over each subinterval I_r, $r=0,1,\ldots,N-1$ as defined in equations (3.2.4) to (3.2.6). As the sensitivity of the extrapolation procedure to round off errors increases with the order of extrapolation, we limit our choice of the order of extrapolation to the range $4\leq m\leq 8$ in all the numerical applications.

Choose h_0, $0<h_0\leq h$ such that

$$\ell = \frac{h}{h_0} \tag{3.3.1}$$

is an integer.

A set of mesh points,

$$\xi_s = x_r + sh, \; s=0,1,\ldots,\ell \tag{3.3.2}$$

are obtained on the interval I_r, $0\leq r\leq N-1$. Equation (3.3.2) gives $\xi_0 = x_r$ and $\xi_\ell = x_{r+1}$.

We now consider a sequence of mesh-sizes defined by

$$\{h_j : h_0 = h;\; h_j = \frac{h_{j-1}}{2} \;,\; j=1,2,\ldots,m\} \tag{3.3.3}$$

where m is the order of extrapolation.

By using the sequence of mesh-sizes given by equation (3.3.3), we can generate a sequence of integers:

$$\{\ell_j : \ell_j = \frac{h}{h_j} \;,\; j=0,1,\ldots,m\}. \tag{3.3.4}$$

If the solution to the initial value problem (3.2.1) at $x = \xi_0$ is given by

$$\underline{y}(\xi_0) = \underline{\beta} \tag{3.3.5}$$

where

$$\underline{\beta} = (\beta_1,\beta_2,\ldots\ldots,\beta_n), \tag{3.3.6}$$

then $y_i(\xi_0) = \beta_i$; $i=1,2,\ldots,n$.

For each component y_i of the solution vector $\underline{y}$, we shall use the sequence of step-lengths given by equation (3.3.3) to generate m+1 estimates of the theoretical solution $y_i(x)$ at $x = x_{r+1}$. These estimates are given by

$$\{y_i(x_{r+1},h_j) \;;\; j=0,1,\ldots,m\} \tag{3.3.7}$$

and it is known that they all have error expansions in powers of h^2. Hence, a suitable linear combination yields the formula

$$\sum_{j=0}^{m} A_{j,m}\, y_i(x_{r+1},h_j) = y_i(x_{r+1}) + O(h^{2m+2}),\quad i=1,2,\ldots,n \tag{3.3.8}$$

where the coefficients of the lower order terms in the error expansion in h^2 have been eliminated. This linear combination of the estimates given by equation (3.3.7) is equivalent (as $m\to\infty$) to extrapolating to h=0 a rational function passing through the points:

$$\{(h_j,y_i(x_{r+1},h_j)),\ j=0,1,\ldots,m\}. \tag{3.3.9}$$

To generate the estimates in equation (3.3.7), Gragg (1964) formulated a modification of the midpoint scheme as follows:

The starting values are obtained as

$$Y_0^i = \beta_i,\ i=1,\ldots,n;\quad Z_0^i = \beta_i + \frac{h_j}{2} f_i(\xi_0,\underline{\beta}),\ i=1,\ldots n \tag{3.3.10}$$

We then evaluate

$$\left.\begin{aligned} Y_{s+1}^i &= Y_s^i + h_j\, f_i(\xi_s + \tfrac{h_j}{2},\underline{Z}_s),\ i=1,\ldots,n \quad \text{and} \\ Z_{s+1}^i &= Z_s^i + h_j\, f_i(\xi_s + h_j,\underline{Y}_{s+1}),\ i=1,\ldots,n; \end{aligned}\right\} \tag{3.3.11}$$

where

$$\underline{Z}_s = (Z_s^1, Z_s^2 \ldots\ldots Z_s^n), \tag{3.3.12}$$

and

$$\underline{Y}_{s+1} = (Y_{s+1}^1, Y_{s+1}^2, \ldots . Y_{s+1}^n) \; . \tag{3.3.13}$$

A smoothing procedure is then carried out at $x = \xi_{\ell_j}$ as follows:

Let

$$U^i(\xi_{\ell_j}, h_j) = Y^i_{\ell_j}, \tag{3.3.14}$$

and

$$P^i(\xi_{\ell_j}, h_j) = Z^i_{\ell_j} - \frac{h_j}{2} f_i(\xi_{\ell_j}, Y_{\ell_j}). \tag{3.3.15}$$

We then obtain the values

$$T^i_j(\xi_{\ell_j}, h_j) = \tfrac{1}{2}[U^i(\xi_{\ell_j}, h_j) + P^i(\xi_{\ell_j}, h_j)]. \tag{3.3.16}$$

Gragg (1964) emphasized that in $T^i_j(\xi_{\ell_j}, h_j)$, the leading unstable component of the discretization error has been eliminated and Stetter (1969) deduced that $T^i_j(\xi_{\ell_j}, h_j)$ is always 'asymptotically strongly stable'. This is consequent upon the smoothing procedure at the end of the subinterval as illustrated by equations (3.3.14) to (3.3.16). Gragg (1964),(1965) showed that $T^i_j(\xi_{\ell_j}, h_j)$ has an error expansion in h^2 i.e.

$$T^i_j(x,h) = y_i(x) + \sum_{s=1}^{m} A^i_s(x) h^{2s} + O(h^{2m+2}) \tag{3.3.17}$$

where the coefficients $A^i_s(x)$, s=1,2,...m are independent of the mesh-size h. Equations (3.3.10) to (3.3.16) are computed for each of the m+1 mesh sizes defined by equation (3.3.3). The quantities $\{T^i_j(\xi_{\ell_j}, h_j),\ j=0,1,\ldots,m\}$ thus obtained will constitute the entries of the first column of the T^i tables illustrated in table (3.3.25). As the quantities in equation (3.3.17) are known to have error expansion in h^2, it is natural to want to obtain a suitable linear combination with the intent to eliminate some of the coefficients in the error terms. This is precisely the essence of the polynomial or rational extrapolation schemes. In most cases, the rational extrapolation scheme as proposed by Bulirsch and Stoer (1966) is more accurate than the polynomial extrapolation proposed by both Aitken (1932) and Neville (1934) (see Joyce,D.C. (1970)). Hence we adapt the rational extrapolation scheme to discontinuous systems of ordinary differential equations.

If we define the functions $S_m^i(h)$, $V_m^i(h)$ as follows:

$$S_m^i(h) = R_{m0}^i(x) + R_{m1}^i(x)\, h^2 + \ldots + R_{mc}^i(x) h^{2c}, \tag{3.3.18}$$

and

$$V_m^i(h) = V_{m0}^i(x) + V_{m1}^i(x) h^2 + \ldots + V_{md}^i(x) h^{2d}, \tag{3.3.19}$$

where

$$c = \left[\frac{m}{2}\right], \text{ the integral part of } \frac{m}{2}$$

and $$d = m-c \tag{3.3.20}$$

then, the rational extrapolation procedure determines a unique rational function

$$R_m^i(h) = \frac{S_m^i(h)}{V_m^i(h)} \tag{3.3.21}$$

which passes through the points $\{(h_j, T_j^i(x_{r+1}, h_j)), j=0,1,\ldots,m\}$.

The rational function $R_m^i(h)$, given by equation (3.3.21) is subject to the following constraints:

$$R_m^i(h_j) = T_m^i(\xi_{\ell_j}, h_j),\ j=0,1,\ldots,m \tag{3.3.22}$$

The extrapolated value $T_{0,m}^i$ at h=0 is then given by

$$
\begin{aligned}
T^i_{0m} &= R^i_m(0) \\
&= T^i_m(x_{r+1},0)
\end{aligned}
\qquad (3.3.23)
$$

which can be computed recursively from equation (3.3.17) by the following algorithm as formulated by Bulirsch and Stoer (1966) i.e.

$$
\begin{aligned}
T^i_{j,-1} &= 0 \\
T^i_{j,0} &= T^i_j(x_{r+1},h_j) \\
T^i_{jk} &= T^i_{j+1,k-1} + \frac{T^i_{j+1,k-1} - T^i_{j,k-1}}{\left(\dfrac{h_j}{h_{j+k}}\right)^2 \left[1 - \dfrac{T^i_{j+1,k-1}-T^i_{j,k-1}}{T^i_{j+1,k-1}-T^i_{j+1,k-2}}\right] - 1}
\end{aligned}
$$

$$
\begin{aligned}
&i=1,2,..,n \\
&j=0,1,..,m \qquad (3.3.24) \\
&k=1,....,m .
\end{aligned}
$$

The last equation in algorithm (3.3.24) connects the elements in position (j,k-1), (j,k),(j+1,k-2) and (j+1,k-1) of the T^i tables in computing the element in the $(j,k)^{th}$ position of the T^i table as illustrated below,

<u>T^i-Table</u>

$$
\begin{array}{llllll}
T^i_{0,0} & T^i_{0,1} & T^i_{0,2} & \cdots\cdots & T^i_{0,m-1} & T^i_{0,m} \\
T^i_{1,0} & T^i_{1,1} & T^i_{1,2} & & T^i_{1,m-1} & \\
T^i_{2,0} & T^i_{2,1} & T^i_{2,2} & \iddots & & \\
\vdots & \vdots & \vdots & & & \\
 & & T^i_{m-2,2} & & & \\
T^i_{m-1,0} & T^i_{m-1,1} & & & & \\
T^i_{m,0} & & & & &
\end{array}
\qquad (3.3.25)
$$

The last m columns of table (3.3.25) are computed with the algorithm (3.3.24). At each step of integration, there are n such tables; one table for each component of the initial value problem.

The following two theorems whose proofs are available in Gragg (1965) give a *necessary and sufficient condition* for the convergence of the algorithm (3.3.24).

Theorem 3.1

A necessary and sufficient condition that

$$\lim_{m\to\infty} T^i_{0m} = y_i(x_{r+1}) \tag{3.3.26}$$

for all functions $T^i_j(x_{r+1},h)$ continuous from the right at $h=0$ is that

$$\sup_{k\geq 0} \frac{h_{k+1}}{h_k} < 1 \tag{3.3.27}$$

where sup represents least upper bound.

Theorem 3.2

If $T^i_j(x_{r+1},h)$ has an error expansion of the form (3.3.17) then as $k\to\infty$

$$T^i_{k,m} - y_i(x_{r+1}) = (-1)^m h_k^2 \ldots\ldots h^2_{k+m}(A^i_{m+1}+0(h_k^2)). \tag{3.3.28}$$

If in addition, we have that

$$\inf \frac{h_{k+1}}{h_k} > 0, \tag{3.3.29}$$

then there exists constants E_m, such that

$$|T^i_{0,m} - y_i(x_{r+1})| < E_{m+1}\, h_k^2 \ldots\ldots h^2_{k+m}. \tag{3.3.30}$$

Whilst equation (3.2.28) states that the entries of each column of table (3.3.25) converges faster to $y_i(x_{r+1})$ than the preceeding column to its left, equation (3.3.30) asserts that the entries of the principal diagonal of the same table converges to $y_i(x_{r+1})$ faster than those of any column. Also equation (3.3.28) gives an estimate of the truncation error at any location of table (3.3.25).

In the next section, we shall consider the convergence criteria of algorithm (3.3.24).

3.4 THE STOPPING CRITERIA FOR THE ALGORITHM (3.2.24)

Let ε denote a specified tolerance and assume that we are computing the k^{th} column of table (3.3.25) for $1 \le k \le m$. Suppose we have just computed the j^{th} (where $1 < j \le m$) element of column k. As an estimate of the truncation error, we obtain the difference e_i as

$$e_i = \frac{|T^i_{j,k} - T^i_{j-1,k}|}{(|T^i_{j-1,k}| + 1)} . \tag{3.4.1}$$

Equation (3.4.1) is in fact an estimate of the mixed error. This choice is simply because mixed error gives a reasonable measure of error for initial value problems with partly small solutions and partly large solutions.

If it is observed that

$$e_i < \varepsilon , \tag{3.4.2}$$

we update the i^{th} component of $\underline{y}(x_{r+1})$ with $T^i_{j-1,k}$ i.e. set

$$y_i(x_{r+1}) = T^i_{j-1,k} . \tag{3.4.3}$$

If the relation (3.4.2) holds for $i=1,2,\ldots,n$, we proceed to the next interval I_{r+1} of integration.

However, if equation (3.4.2) is violated by at least one component $y_s(x_{r+1})$ say of $\underline{y}(x_{r+1})$ i.e.

$$|T^s_{0,m} - T^s_{1,m-1}| > \varepsilon(|T^s_{1,m-1}| + 1) , \tag{3.4.4}$$

we increase the order of extrapolation m by two if the current order m<8 and repeat the integration procedure in the interval I_r. However, if the current order of extrapolation is the maximum allowed (i.e. m=8 for our case), we repeat the integration procedure in the interval I_r with smaller stepsize.

It is usual to halve the stepsize.

It is possible that we shall encounter a point of discontinuity within the interval I_r. The next section deals with methods of coping with such a situation.

3.5 The Treatment of Discontinuities

In this section, we shall obtain a sequence of subintervals $\{I_{r,\lambda}, \lambda = 0,1,\ldots\}$ which contracts to the point of discontinuity.

If $L(I_{r,\lambda})$ denotes the length of the subinterval $I_{r,\lambda}$ with $I_{r,0} = I_r$, then

$$L(I_{r,0}) = h. \tag{3.5.1}$$

For $\lambda>0$, we shall obtain the result

$$L(I_{r,\lambda}) = 2^{-\lambda m}.L(I_{r,0})$$

$$= 2^{-\lambda m}.h. \tag{3.5.2}$$

The occurrence of any discontinuity in the interval I_r given by

$$x_r \leq x \leq x_{r+1}, \quad r=0,1,\ldots,N-1$$

is detected with the change in the sign of the discontinuity function $\gamma=\gamma(x,\underline{y})$. In obtaining the elements of the first column of the T^i-tables given by equation (3.3.25), we first generate the last elements i.e. the vector $\underline{T}_m$ given by

$$\underline{T}_m = (T^1_{m,0}, T^2_{m,0}, \ldots, T^n_{m,0}) \tag{3.5.3}$$

rather than the first element $\underline{T}_0$ given by

$$\underline{T}_0 = (T^1_{00}, T^2_{00}, \ldots, T^n_{00}). \tag{3.5.4}$$

This approach saves n function evaluations if there is a point of discontinuity in the interval I_r. The computation of the vector $\underline{T}_m$, given by equation (3.5.3) entails a division of the interval I_r into 2^m equal subintervals:

$$x_r = \xi_0 < \xi_1 < \xi_2 < \ldots\ldots < \xi_{\ell_m} = x_{r+1} = x_r + h \tag{3.5.5}$$

i.e.,

$$\xi_j = \xi_0 + j.h_m\ ,\ j=0,1,\ldots \ell_m \tag{3.5.6}$$

with h_m given by equation (3.3.3) and ℓ_m given by equation (3.3.4).

The existence of a point of discontinuity in the interval I_r is indicated by the following relation:

$$\gamma(\xi_0,\underline{\beta}) \cdot \gamma(\xi_{\ell_m},\underline{T}_m) \leqslant 0 \tag{3.5.7}$$

with $\underline{\beta}$ defined by equation (3.3.6) and $\underline{T}_m$ defined by equation (3.5.3).

If the relation (3.5.7) holds, we now try to locate the point of discontinuity in one of the subintervals

$$\{u_i : u_i = \xi_i \leqslant x \leqslant \xi_{i+1}, \quad i=0,1,\ldots\ell_m-1\} \quad . \tag{3.5.8}$$

Clearly, we observe that the interval I_r relates to the subintervals u_i, i=0,1,...,m-1 as follows:

$$I_r = \bigcup_{i=0}^{\ell_m -1} u_i \quad . \tag{3.5.9}$$

Let the vector $\underline{Z}^*_s$ be defined by

$$\underline{Z}^*_s = (Y^1_s, Y^2_s, \ldots, Y^n_s) \tag{3.5.10}$$

whose elements are obtained by equations (3.3.10) and (3.3.11).

We then obtain s* as

$$s^* = \min_s \{s : \gamma(\xi_0,\underline{\beta}) \cdot \gamma(\xi_s,\underline{Z}^*_s) \leqslant 0, \quad s=1,2,\ldots\ell_m\} \quad . \tag{3.5.11}$$

If we define t* by

$$t^* = s^*-1 \tag{3.5.12}$$

equation (3.5.11) indicates that the point of discontinuity lies within the subinterval

$$u_{t^*} = \xi_{t^*} \leqslant x \leqslant \xi_{s^*} \quad . \tag{3.5.13}$$

The normal integration procedure is now carried out over the interval I^*_r defined by

$$I^*_r = \xi_0 \leqslant x \leqslant \xi_{t^*} \quad . \tag{3.5.14}$$

Thus we have succeeded in confining the point of discontinuity to within the interval

$$I_{r,1} = u_t^* \tag{3.5.15}$$

defined by equation (3.5.13). The length of the interval is given as

$$\begin{aligned} L(I_{r,1}) &= h_m \\ &= 2^{-m}h \ . \end{aligned} \tag{3.5.16}$$

The interval $I_{r+1} = x_r \leq x \leq x_{r+1}$ is now replaced by the interval $I_{r,1}$ given by equations (3.5.15) and (3.5.13) and the mesh size h is replaced by h_m.

As it is clearly evident that the new subinterval I_{r+1} contains a point of dicsontinuity, the process (3.5.1) to (3.5.16) is repeated to generate

$$I_{r,2},\ I_{r,3},\ldots,\text{etc.}$$

At the k^{th} iteration, we obtain the interval $I_{r,k}$ of length

$$L(I_{r,k}) = 2^{-mk}.h$$

It is obvious that

$$\lim_{k\to\infty} L(I_{r,k}) = 0$$

and hence the sequence $\{I_{r,k}\}$ thus generated converges to the point of discontinuity from the left.

For instance with an initial step size h=1, and order of extrapolation m=6, the point of discontinuity is located correctly to within an accuracy of

$$\begin{aligned} 2^{-mk} &= 2^{-(4)(6)} \\ &= 2^{-24} \\ &\simeq 10^{-7} \end{aligned}$$

in four iterations.

3.6 COMPUTATIONAL RESULTS

Example 3.6.1

We first consider the scalar initial value problem

$$\frac{dy}{dx} = \left[-(x+y)+2\sqrt{2}\right]^{\frac{1}{2}} \tag{3.6.1a}$$

$$y(0) = 0$$

over the interval $0 \leqslant x \leqslant 2$.

The discontinuity condition is given by

$$\gamma(x,y) = y^2-2 \quad . \tag{3.6.1b}$$

The numerical integration procedure was implemented with uniform mesh size $h=0.13$ and the order of extrapolation allowed to vary in the range $6 \leqslant m \leqslant 8$. The allowable tolerance is $\varepsilon = 10^{-8}$.

As can be observed in table (3.6.1) below, the point of discontinuity is located as

$$(x=1.2882992 \;, \quad y = 1.4142135)$$

in four iterations.

TABLE 3.6.1

ORDER OF EXTRAPOLATION	X	Y	$10^8 x T_{t+1}$
6	0.0000000	0.0000000	0.00000
8	0.1300000	0.2118423	0.58899
8	0.2600000	0.4098710	0.65374
8	0.3900000	0.5936920	0.73196
8	0.5200000	0.7628328	0.83964
8	0.6500000	0.9167143	0.98153
8	0.7800000	1.0546044	0.29395
8	0.9100000	1.1755377	0.37398
8	1.0400000	1.2781610	0.48749
8	1.1700000	1.3603783	0.76689
8	1.2878125	1.4140406	0.91822
6	1.2882886	1.4142098	0.00000
6	1.2882990	1.4142135	0.00146
6	1.2882992	1.4142135	0.01746

Example 6.3.2

We now consider the case of an inelastic body falling freely under gravity. It is dropped from a height of 64 feet above the ground. We wish to determine its velocity when it reaches the ground as well as the duration of motion.

Let g denote the acceleration due to gravity where $g = 32$ feet/sec^2. The problem can be formulated as follows:

Let $\underline{y}=(y_1,y_2)^T$ and the range of integration is $0 \leq x < \infty$.

If, y_1 denotes the height and y_2 the velocity, then we obtain the initial value problem

$$\frac{d}{dx}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} 0 \\ g \end{pmatrix}, \tag{3.6.2a}$$

where

$$\begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix} = \begin{pmatrix} 64 \\ 0 \end{pmatrix} . \tag{3.6.2b}$$

We define the discontinuity function as

$$\gamma(x,\underline{y}) = y_1^2 . \tag{3.6.2c}$$

Details of the numerical results are given in table (3.6.2) below. The point of discontinuity was obtained at $x = 2$, $y_1 = 0$, $y_2 = 64$.

Hence a body falling freely under the gravitational acceleration from a height of 64 feet reaches the ground after two seconds with a velocity of 64 feet/second.

TABLE 3.6.2

ORDER OF EXTRAPOLATION	X	Y_1	Y_2	$10^{10} x T^{(1)}_{t+1}$	$10^{10} x T^{(2)}_{t+1}$
8	0.0000000	64.0000000	0.0000000	0.00000	0.00000
8	0.3300000	62.2576000	10.5600000	0.07480	0.00000
8	0.6600000	57.0304000	21.1200000	0.00000	0.11024
8	0.9900000	48.3184000	31.6800000	0.00000	0.00000
8	1.3200000	36.1216000	42.2400000	0.00000	0.11024
8	1.6500000	20.4400000	52.8000000	0.00000	0.08819
8	1.9800000	1.2736000	62.3600000	1.02832	0.07349
8	1.9993359	0.0424929	63.9787500	0.00000	0.07278
8	1.9999956	0.0002832	63.9998580	0.00121	0.00000
8	2.0000000	0.0000000	64.0000000	0.00000	0.07276

Example 3.6.3

We finally considered the scalar problem

$$y' = \begin{cases} x & 0 \leqslant x \leqslant 0.5 \\ 1-x & 0.5 \leqslant x \leqslant 1.0 \end{cases} \tag{3.6.3a}$$

with initial condition

$$y(0) = 0 \tag{3.6.3b}$$

over the range $0 \leqslant x \leqslant 1$.

The discontinuity condition is specified as

$$\gamma(x,y) = \begin{cases} y & 0 \leqslant x \leqslant 0.5 \\ -y & 0.5 \leqslant x \leqslant 1 \end{cases}$$

The system (3.6.3a) is continuous but does not have a continuous derivative. Hence it violates the conditions of theorem (1.1).

The point of discontinuity was located at the point ($x=0.5$, $y=0.125$).

Details of the numerical results are given in table (3.6.3) below. In this example, we integrate beyond the point of discontinuity.

TABLE 3.6.3

ORDER OF EXTRAPOLATION	H	X	Y	$10^8 x T_{t+1}$
6	0.13000000	0.00000000	0.00000000	0.00000
6	0.13000000	0.13000000	0.00845000	0.00000
6	0.13000000	0.26000000	0.03380000	0.00000
6	0.13000000	0.39000000	0.07605000	0.07654
6	0.10968750	0.49968749	0.12484379	0.13987
6	0.00028564	0.49997314	0.12498657	0.09314
6	0.00002678	0.49999992	0.12499996	0.09313
6	0.00000007	0.50000000	0.12500000	0.00000
6	0.13000000	0.63000000	0.18155000	0.06412
6	0.13000000	0.76000000	0.22120000	0.05263
6	0.13000000	0.89000000	0.24395000	0.00000
6	0.10999999	1.00000000	0.24999999	0.18626

3.7 CONCLUSION

This approach locates the point of discontinuity to any desired accuracy in a geometric progression with common ratio 2^{-m}, $(4 \leq m \leq 8)$ where m is the order of extrapolation.

However, the scheme is liable to fail if the point of discontinuity is a local minimum or maximum of the solution vector.

CHAPTER IV

A VARIABLE ORDER ONE-STEP ALGORITHM FOR THE NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS WITH OSCILLATORY SOLUTIONS

4.1 Introduction

In Lambert and Shaw (1966), a class of two-point formulae for the numerical solution of the initial value problem

$$y' = f(x,y),\ y(x_0) = y_0 \qquad (4.1.1)$$

whose solutions may contain singularities is introduced.

These formulae are based on the representation of the solution to the initial value problem (4.1.1) by a non-polynomial interpolant (2.6.1) which contains two real parameters which are automatically chosen and revised as the computation progresses. These parameters generally converge to some suitable values which are used to re-integrate the given system. The parameters control the position and nature of the singularities in the solution to the problem (4.1.1).

In this chapter, an alternative strategy is outlined in which new integration formulae are developed by representing the solution to (4.1.1) by a combination of a polynomial and trigonometric or hyperbolic interpolant. Each interpolant contains two real parameters which are accurately determined numerically at each step of integration. The algorithm is adaptive in the sense that we automatically vary the degree of the polynomial part of the interpolant or switch from trigonometric interpolant to hyperbolic interpolant (or vice versa) accordingly as the need arises. In the practical cases investigated, polynomial orders of one or two were found sufficient to obtain reasonable accuracy.

As our approach is component applicable to systems of ordinary differential equations, we shall derive the integration formulae for the scalar case for the sake of clarity. However, the practical applications include systems of ordinary differential equations.

4.2 DEFINITION OF THE LOCAL INTERPOLANT

We shall consider the initial value problem of the form

$$y' = f(x,y) \ , \ y(a) = \eta \tag{4.2.1}$$

An integer N is chosen to define a uniform mesh-size h as

$$h = \frac{b-a}{N}. \tag{4.2.2}$$

A sequence of mesh-points is then defined as

$$\{x_t : x_t = a+th, \ t=0,1,\ldots,N\} . \tag{4.2.3}$$

If we define the subintervals $\{I_t\}$ such that:

$$I_t = x_t \leq x \leq x_{t+1}, \ t=0,1,\ldots,N-1; \tag{4.2.4}$$

then the interval $I = a \leq x \leq b$ can be expressed as:

$$I = \bigcup_{t=0}^{N-1} I_t . \tag{4.2.5}$$

Equation (4.2.5) is a division of interval I into N equal subintervals.

On every subinterval I_t, we assume that the solution to the initial value problem (4.2.1) is locally represented by the interpolant

$$F_t(x) = \sum_{r=0}^{L} a_r x^r + b_t \sin(N_t x + A_t) \ , \ a_L \neq 0 \tag{4.2.6}$$

where the integer $L > 0$ is the degree of the polynomial part of the interpolant; b_t and $(a_r, r=0,1,\ldots,L)$ are real undetermined coefficients whilst N_t and A_t are real parameters to be accurately determined at each step of integration.

Let us define the polynomial $P_t(x)$ by;

$$E_t(x) = \sum_{r=0}^{L} a_r x^r \tag{4.2.7}$$

and the function $Q_t(x)$ by;

$$Q_t(x) = \sin(N_t x + A_t) . \tag{4.2.8}$$

The interpolant (4.2.6) is then given by

$$F_t(x) = E_t(x) + b_t Q_t(x) . \tag{4.2.9}$$

4.3 DERIVATION OF THE INTEGRATION FORMULAE

Let the numerical solution to the initial value problem (4.2.1) at $x=x_t$ be y_t and the theoretical solution be $y(x_t)$.

Under the assumption that the function $f=f(x,y)$ belongs to the class $C^{\infty}[a,b]$, we impose the following constraints on the interpolating function (4.2.6):

(a) That the interpolant assumes the solution to (4.2.1) at the points $x = x_t$ and $x = x_{t+1}$, i.e.

$$F_t(x_t) = y_t \quad , \tag{4.3.1}$$

and

$$F_t(x_{t+1}) = y_{t+1} \quad . \tag{4.3.2}$$

(b) That the first and higher order derivatives of the interpolant coincide with the function $f=f(x,y)$, its first and higher derivatives up to the $(L+1)^{th}$ derivative at the point $x = x_t$, i.e.

$$\frac{d^s}{dx^s}\Big[F_t(x)\Big]_{x=x_t} = \frac{d^{s-1}}{dx^{s-1}}\Big[f(x,y)\Big]_{\substack{x=x_t\\ y=y_t}}$$

$$= \frac{\partial f^{(s-2)}(x,y)}{\partial x} + f(x,y)\,\frac{\partial f^{(s-2)}(x,y)}{\partial y}\Bigg|_{\substack{x=x_t\\ y=y_t}}$$

$$s=1,2,\ldots L+1 \; . \tag{4.3.3}$$

The constraints (4.3.1) to (4.3.3) will suffice to eliminate the undetermined coefficients. For the sake of clarity, we shall give details of the derivation of the integration formula for the case when the polynomial part of the interpolant $E_t(x)$ is of degree one (i.e. $L=1$). We shall state the results for the cases when degree L of $E_t(x)$ the polynomial part of the interpolating function (4.2.6) is greater than one.

By imposing the constraints (4.3.1) and (4.3.2) on the interpolant (4.2.6) we obtain the following formulae:

$$y_t = a_0 + a_1 x_t + b_t \sin(N_t x_t + A_t) \tag{4.3.4}$$

and

$$y_{t+1} = a_0 + a_1 x_{t+1} + b_t \sin(N_t x_{t+1} + A_t) \,. \tag{4.3.5}$$

By subtracting equation (4.3.4) from equation (4.3.5) and applying equation (4.2.3), we have the relation:

$$y_{t+1} - y_t = a_1 h + b_t \left[\sin((N_t x_t + A_t) + N_t h) - \sin(N_t x_t + A_t)\right] . \tag{4.3.6}$$

The immediate objective is to rid equation (4.3.6) of the remaining undetermined coefficients (i.e. a_1 and b_t). If the constraint (4.3.3) is now imposed on equation (4.2.6) we obtain:

$$f(x_t, y_t) = a_1 + N_t b_t \cos(N_t x_t + A_t) \,, \tag{4.3.7}$$

and

$$f^{(1)}(x_t, y_t) = -N_t^2 \, b_t \, \sin(N_t x_t + A_t) \,, \tag{4.3.8}$$

Equation (4.3.8) implies that:

$$b_t = \frac{-f^{(1)}(x_t, y_t)}{N_t^2 \sin(N_t x_t + A_t)} \,, \tag{4.3.9}$$

and using equation (4.3.9) in equation (4.3.7) gives the relationship:

$$a_1 = \left[f(x_t, y_t) + \frac{f^{(1)}(x_t, y_t)}{N_t} \cot(N_t x_t + A_t)\right] . \tag{4.3.10}$$

We can now use equations (4.3.9) and (4.3.10) to eliminate the undetermined coefficients b_t and a_1 from equation (4.3.6) to yield:

$$y_{t+1} = y_t + hf(x_t, y_t) + \frac{h}{N_t} f^{(1)}(x_t, y_t) \cot(N_t x_t + A_t)$$

$$- \frac{f^{(1)}(x_t,y_t)}{N_t^2 \sin(N_t x_t + A_t)} \cdot \left[\sin((N_t x_t + A_t) + N_t h) - \sin(N_t x_t + A_t)\right] \cdot \tag{4.3.11}$$

By using similar arguments as in procedure (4.3.4) to (4.3.10) we obtain the following formulae when the polynomial part of the interpolant (4.2.6) are as follows:

For $E_t(x)$ of degree 2 i.e. (L=2)

$$y_{t+1} = y_t + hf(x_t,y_t) + \frac{h^2}{2} f^{(1)}(x_t,y_t) - \frac{h^2}{2N_t^2} f^{(2)}(x_t,y_t) \tan(N_t x_t + A_t) - \frac{f^{(2)}(x_t,y_t)}{N_t^3 \cos(N_t x_t + A_t)} \cdot \left[\sin((N_t x_t + A_t) + N_t h) - \sin(N_t x_t + A_t)\right] \tag{4.3.12}$$

For $E_t(x)$ of degree 3 (i.e. L=3)

$$y_{t+1} = y_t + hf(x_t,y_t) + \frac{h^2}{2} f^{(1)}(x_t,y_t) + \frac{h^3}{6} f^{(2)}(x_t,y_t) - \frac{h}{N_t^3} f^{(3)}(x_t,y_t) \cot(N_t x_t + A_t) + \frac{h^2}{2N_t} f^{(3)}(x_t,y_t) - \frac{f^{(3)}(x_t,y_t)}{N_t^4 \sin(N_t x_t + A_t)} \cdot \left[\sin((N_t x_t + A_t) + N_t h) - \sin(N_t x_t + A_t)\right] \tag{4.3.13}$$

and finally,

For $E_t(x)$ of degree 4 (i.e. L=4)

$$y_{t+1} = y_t + \sum_{i=1}^{4} \frac{h^i}{i!} f^{(i-1)}(x_t,y_t) - \frac{h}{N_t^4} f^{(4)}(x_t,y_t) + \frac{h^2}{2N_t^3} f^{(4)}(x_t,y_t) \tan(N_t x_t + A_t) + \frac{h^3}{6N_t^2} f^{(4)}(x_t,y_t)$$

$$- \frac{h^4}{24N_t} f^{(4)}(x_t,y_t)\tan(N_t x_t+A_t)$$

$$+\frac{f^4(x_t,y_t)}{N_t^5\cos(N_t x_t+A_t)} \cdot \left[\sin((N_t x_t+A_t)+N_t h)-\sin(N_t x_t+A_t)\right] \cdot \tag{4.3.14}$$

In equations (4.3.11) to (4.3.14), the parameters N_t and A_t are still to be determined. Their values will be obtained in the next section.

4.4 DETERMINATION OF THE PARAMETERS N_T AND A_T AND TRUNCATION ERRORS

In this section, we shall obtain the error expansions in h for the one-step integration formulae given by equations (4.3.11) to (4.3.14). The parameters N_t and A_t are then obtained by ensuring that the first two terms in these error expansions vanish. As in the previous section, we shall give detailed arguments when the polynomial $\varepsilon_t(x)$ of the interpolating function is linear in x (i.e. L=1).

If the numerical solution y_{t+1} approximates the theoretical solution $y(x_{t+1})$ at $x=x_{t+1}$, with $x_{t+1} = x_t+h$, the Taylor's series expansion for $y(x_{t+1})$ at $x=x_t$ yields:

$$y(x_{t+1}) = y(x_t+h)$$

$$= y_t + \sum_{s=1}^{\infty} \frac{h^s}{s!} f^{(s-1)}(x_t,y_t) \quad . \quad (4.4.1)$$

The usual trigonometric addition formulae give the following relationship i.e.

$$\sin((N_tx_t+A_t)+N_th) = \sin(N_tx_t+A_t)\cos(N_th) + \cos(N_tx_t+A_t)\sin(N_th) \quad . \quad (4.4.2)$$

Also, the Maclaurin's series gives:

$$\cos(N_th) = \sum_{i=0}^{\infty} (-1)^i \frac{(N_th)^{2i}}{(2i)!} \quad (4.4.3)$$

and

$$\sin(N_th) = \sum_{i=0}^{\infty} (-1)^i \frac{(N_th)^{2i+1}}{(2i+1)!} \quad . \quad (4.4.4)$$

The truncation error at $x = x_{t+1}$ is denoted by T_{t+1} and is defined as the difference between the numerical solution and the theoretical solution, i.e.

$$T_{t+1} = y(x_{t+1}) - y_{t+1} \quad . \quad (4.4.5)$$

If we now substitute equations (4.3.11) and (4.4.1) in equation (4.4.5), we obtain the following expression for the truncation error:

$$T_{t+1} = \left[y(x_t) + \sum_{s=1}^{\infty} \frac{h^s}{s!} f^{(s-1)}(x_t,y_t)\right] - \{y_t + hf(x_t,y_t)$$

$$+ \frac{h}{N_t} f^{(1)}(x_t,y_t)\cot(N_t x_t + A_t)$$

$$- \frac{f^{(1)}(x_t,y_t)}{N_t^2 \sin(N_t x_t + A_t)} \cdot \left[\sin((N_t x_t + A_t) + N_t h)\right.$$

$$\left. - \sin(N_t x_t + A_t)\right]\} \quad . \qquad (4.4.6)$$

By making the simplifying assumption that there is no previous error (i.e. that $y(x_t) = y_t$), then the truncation error T_{t+1} at $x = x_{t+1}$ given by equation (4.4.6) can be expressed as follows:

$$T_{t+1} = \sum_{s=2}^{\infty} \frac{h^s}{s!} f^{(s-1)}(x_t,y_t) - \frac{h}{N_t} f^{(1)}(x_t,y_t)\cot(N_t x_t + A_t)$$

$$+ \frac{f^{(1)}(x_t,y_t)}{N_t^2 \sin(N_t x_t + A_t)} \left[\sin((N_t x_t + A_t) + N_t h)\right.$$

$$\left. - \sin(N_t x_t + A_t)\right] \quad . \qquad (4.4.7)$$

By using the relationship (4.4.2) in (4.4.7) we have

$$T_{t+1} = \sum_{s=2}^{\infty} \frac{h^s}{s!} f^{(s-1)}(x_t,y_t) - \frac{h}{N_t} f^{(1)}(x_t,y_t)\cot(N_t x_t + A_t)$$

$$+ \frac{f^{(1)}(x_t,y_t)}{N_t^2}\cos(N_t h) + \frac{f^{(1)}(x_t,y_t)}{N_t^2}\cot(N_t x_t + A_t) \times$$

$$\sin(N_t h) - \frac{f^{(1)}(x_t,y_t)}{N_t^2} \quad . \qquad (4.4.8)$$

As we are interested in an error expansion in the mesh size h, we use the identities (4.4.3) and (4.4.4) in equation (4.4.8) to yield

$$T_{t+1} = \sum_{s=2}^{\infty} \frac{h^s}{s!} f^{(s-1)}(x_t,y_t) + \frac{h}{N_t} f^{(1)}(x_t,y_t)\cot(N_t x_t+A_t)$$

$$- \frac{f^{(1)}(x_t,y_t)}{N_t^2} \left[\sum_{i=0}^{\infty} (-1)^i \frac{(N_t h)^{2i}}{(2i)!}\right]$$

$$- \frac{f^{(1)}(x_t,y_t)}{N_t^2} \cot(N_t x_t+A_t) \left[\sum_{i=0}^{\infty} (-1)^i \frac{(N_t h)^{2i+1}}{(2i+1)!}\right] +$$

$$\frac{f^{(1)}(x_t,y_t)}{N_t^2} . \qquad (4.4.9)$$

Equation (4.4.9) thus expresses the truncation error at $x=x_{t+1}$ as a polynomial in the mesh-size h. By ensuring that the first two terms in the error expansion in h vanish, we obtain the values of the parameters N_t and A_t as:

$$N_t = \left[\frac{-f^{(3)}(x_t,y_t)}{f^{(1)}(x_t,y_t)}\right]^{\frac{1}{2}} \qquad (4.4.10)$$

and

$$A_t = \cot^{-1}\left[\frac{f^{(2)}(x_t,y_t)}{N_t f^{(1)}(x_t,y_t)}\right] - N_t x_t . \qquad (4.4.11)$$

The truncation error is now expressed as:

$$T_{t+1} = \sum_{s=3}^{\infty} \frac{h^{2s}}{(2s)!} \left[f^{(2s-1)}(x_t,y_t)+(-1)^s N_t^{2s-2} f^{(1)}(x_t,y_t)\right]$$

$$+ \sum_{s=2}^{\infty} \frac{h^{2s+1}}{(2s+1)!} \left[f^{(2s)}(x_t,y_t) +(-1)^s N_t^{2s-1} f^{(2)}(x_t,y_t)\right] .$$

(4.4.12)

In general, for an arbitrary degree L of the polynomial $E_t(x)$ in the interpolant (4.2.6), the parameters N_t and A_t are given by;

$$N_t = \left(\frac{-f^{(L+2)}(x_t,y_t)}{f^{(L)}(x_t,y_t)} \right)^{\frac{1}{2}} \tag{4.4.13}$$

and either

$$A_t = \cot^{-1}\left(\frac{f^{(L+1)}(x_t,y_t)}{N_t f^{(L)}(x_t,y_t)} \right) - N_t x_t \tag{4.4.14}$$

when L is odd or

$$A_t = \tan^{-1}\left(\frac{-f^{(L+1)}(x_t,y_t)}{N_t f^{(L)}(x_t,y_t)} \right) - N_t x_t \tag{4.4.15}$$

when L is even.

By using equations (4.4.13) to (4.4.15) in the truncation errors, they are finally expressed as follows:

<u>When $\varepsilon_t(x)$ is of degree L=1,</u>

$$T_{t+1} = \sum_{s=L+2}^{\infty} \frac{h^{2s}}{(2s)!} \left[f^{(2s-1)}(x_t,y_t) + (-1)^s N_t^{\,2s-L-1} f^{(L)}(x_t,y_t) \right] + \sum_{s=L+1}^{\infty} \frac{h^{2s+1}}{(2s+1)!} \left[f^{(2s)}(x_t,y_t) + (-1)^s N_t^{\,2s-L-1} f^{(L+1)}(x_t,y_t) \right] \tag{4.4.16}$$

<u>When $\varepsilon_t(x)$ is of degree L=2</u>

$$T_{t+1} = \sum_{s=L+1}^{\infty} \frac{h^{2s+1}}{(2s+1)!} \left[f^{(2s)}(x_t,y_t) + (-1)^s N_t^{\,2s-L} f^{(L)}(x_t,y_t) \right] + \sum_{s=L+1}^{\infty} \frac{h^{2s}}{(2s)!} \left[f^{(2s-1)}(x_t,y_t) + (-1)^{s+1} N_t^{2s-L-2} f^{(L+1)}(x_t,y_t) \right] \tag{4.4.17}$$

<u>When $\varepsilon_t(x)$ is of degree L=3</u>

$$T_{t+1} = \sum_{s=L+1}^{\infty} \frac{h^{2s}}{(2s)!} \left[f^{(2s-1)}(x_t,y_t) + (-1)^{s+1} N_t^{2s-L-1} f^{(L)}(x_t,y_t) \right] + \sum_{s=L}^{\infty} \frac{h^{2s+1}}{(2s+1)!} \left[f^{(2s)}(x_t,y_t) + (-1)^{s+1} N_t^{2s-L-1} f^{(L+1)}(x_t,y_t) \right] \tag{4.4.18}$$

and finally

When $E_t(x)$ is of degree L=4

$$T_{t+1} = \sum_{s=L}^{\infty} \frac{h^{2s+1}}{(2s+1)!} \left[f^{(2s)}(x_t,y_t)+(-1)^{s+1}N_t^{\,2s-L}f^{(L)}(x_t,y_t)\right]$$

$$+ \sum_{s=L}^{\infty} \frac{h^{2s}}{(2s)!} \left[f^{(2s-1)}(x_t,y_t)+(-1)^{s}N_t^{\,2s-L-2}f^{(L+1)}(x_t,y_t)\right].$$

(4.4.19)

4.5 FINAL INTEGRATION FORMULAE

In this section, we shall use the Maclaurin's series expansion for $\cos(N_t h)$ and $\sin(N_t h)$ given by equations (4.4.3) and (4.4.4), the trigonometric addition formula given by equation (4.4.2) as well as the expressions for the parameters N_t and A_t as given in equations (4.4.13) to (4.4.15) to obtain the final integration formula for the case when $\mathcal{E}_t(x)$ is of degree one.

From equation (4.4.14), we have

$$\cot(N_t x_t + A_t) = \frac{f^{(L+1)}(x_t,y_t)}{N_t f^{(L)}(x_t,y_t)} . \tag{4.5.1}$$

By using the addition formula given by equation (4.3.2); and equations (4.5.1),(4.4.13),(4.4.3) and (4.4.4) in the integration formula given by equation (4.3.11), the final integration formula is given by:

$$y_{t+1} = y_t + hf(x_t,y_t) - \frac{f^{(1)}}{N_t^2}(x_t,y_t)\left[\cos(N_t h) - 1\right]$$
$$- \frac{f^{(2)}(x_t,y_t)}{N_t^3}\left[\sin(N_t h) - N_t h\right] . \tag{4.5.2}$$

The final integration formulae for higher degrees of the polynomial $\mathcal{E}_t(x)$ are given as follows;

When $\mathcal{E}_t(x)$ is of degree L=2, we have:

$$y_{t+1} = y_t + \sum_{r=1}^{L} \frac{h^r}{r!} f^{(r-1)}(x_t,y_t)$$
$$+ \frac{f^{(3)}(x_t,y_t)}{N_t^4}\left\{\cos(N_t h) - \left[1 - \frac{(N_t h)^2}{2}\right]\right\}$$

$$- \frac{f^{(2)}(x_t,y_t)}{N_t^3} \left[\sin(N_t h)-N_t h\right] \qquad (4.5.3)$$

When $\mathcal{E}_t(x)$ is cubic (i.e. L=3), we have

$$y_{t+1} = y_t + \sum_{r=1}^{L} \frac{h^r}{r!} f^{(r-1)}(x_t,y_t)$$

$$+ \frac{f^{(3)}(x_t,y_t)}{N_t^4} \{\cos(N_t h) - [1-\frac{(N_t h)^2}{2!}]\}$$

$$+ \frac{f^{(4)}}{N_t^5} \{\sin(N_t h) - [N_t h- \frac{(N_t h)^3}{3!}]\} \qquad (4.5.4)$$

and finally

When the polynomial $\mathcal{E}_t(x)$ is of degree four (i.e. L=4), we have

$$y_{t+1} = y_t + \sum_{r=1}^{L} \frac{h^r}{r!} f^{(r-1)}(x_t,y_t)$$

$$+ \frac{f^{(4)}(x_t,y_t)}{N_t^5} \{\sin(N_t h)-[N_t h- \frac{(N_t h)^3}{3!}]\}$$

$$- \frac{f^{(5)}(x_t,y_t)}{N_t^6} \{\cos(N_t h) - [1- \frac{(N_t h)^2}{2!} + \frac{(N_t h)^4}{4!}]\} . \qquad (4.5.5)$$

With the definition (2.3.1) and the formulae for the truncation errors given by equations (4.4.16) to (4.4.19) we establish the following relation between the degree L of the polynomial $\mathcal{E}_t(x)$ in the interpolating function (4.2.6) and the order p of the corresponding integration formulae given by equations (4.5.2) to (4.5.5).

L	p
1	4
2	5
3	6
4	7

(4.5.6)

In general, we conclude that if the degree of the polynomial $\mathcal{E}_t(x)$ in the interpolating function (4.2.6) is L, the resulting integration formula is of order p given by the relation:

$$p = L + 3 . \tag{4.5.7}$$

4.6 STABILITY OF THE INTEGRATION FORMULAE

In this section, we shall investigate the stability properties of the integration formulae given by equations (4.5.2) to (4.5.5). We shall give details for only the scheme of order four as the argument for the higher order schemes follows an identical pattern.

By re-introducing the Maclaurin's series expansions for $\sin(N_t h)$ and $\cos(N_t h)$ equation (4.5.2) gives

$$y_{t+1} = y_t + hf(x_t,y_t) - h^2 f^{(1)}(x_t,y_t)\left(\sum_{i=1}^{\infty}(-1)^i \frac{(N_t h)^{2i-2}}{(2i)!}\right) - h^3 f^{(2)}(x_t,y_t)\left(\sum_{i=1}^{\infty}(-1)^i \frac{(N_t h)^{2i-2}}{(2i+1)!}\right). \tag{4.6.1}$$

We now define the increment function $\phi = \phi(x,y;h)$ of the one-step integration formula (4.5.2) as

$$\phi(x,y;h) = f(x,y) - hf^{(1)}(x,y)\left(\sum_{i=1}^{\infty}(-1)^i \frac{(N_t h)^{2i-2}}{(2i)!}\right) - h^2 f^{(2)}(x,y)\left(\sum_{i=1}^{\infty}(-1)^i \frac{(N_t h)^{2i-2}}{(2i+1)!}\right). \tag{4.6.2}$$

The fourth order integration scheme given by equation (4.6.1) can then be expressed as

$$y_{t+1} = y_t + h\phi(x_t,y_t;h), \tag{4.6.3}$$

with the increment function $\phi(x,y;h)$ given by equation (4.6.2). Equation (4.6.3) is the normal form for the one step scheme for solving initial value problems in ordinary differential equations.

Lemma 4.1

If the function $f=f(x,y) \varepsilon C^{\infty}[a,b]$, then $f(x,y), f^{(1)}(x,y)$ and $f^{(2)}(x,y)$ satisfy *a* Lipschitz condition.

Proof

If $f = f(x,y) \varepsilon C^{\infty}[a,b]$, then for (x,y) and (x,y^*) in R, the mean value theorem gives

$$f(x,y) - f(x,y^*) = \frac{\partial f}{\partial y}(x,\bar{y})(y-y^*) \tag{4.6.4}$$

where $(x,\bar{y})$ is within the interval defined by the points (x,y) and (x,y^*). We can now choose L_* such that

$$L_* = \sup_{(x,y)\varepsilon R} \left| \frac{\partial f(x,y)}{\partial y} \right| < \infty \quad . \tag{4.6.5}$$

By taking the norm of both sides of equation (4.6.4) and applying equation (4.6.5) we have

$$|f(x,y) - f(x,y^*)| = \left|\frac{\partial f(x,\bar{y})}{\partial y}(y-y^*)\right| \leq L_*|y-y^*| \; . \tag{4.6.6}$$

We have thus established that $f(x,y) \varepsilon C^{\infty}[a,b]$ implies that $f(x,y)$ satisfies the Lipschitz condition. Since $f(x,y) \varepsilon C^{\infty}[a,b]$, then $f^{(1)}(x,y) \varepsilon C^{\infty}[a,b]$ and this in turn implies that $f^{(2)}(x,y) \varepsilon C^{\infty}[a,b]$. By using similar arguments for $f^{(1)}(x,y)$ and $f^{(2)}(x,y)$ as those for $f(x,y)$, we can obtain constants $L_1<\infty$ and $L_2<\infty$ such that,

$$|f^{(1)}(x,y) - f^{(1)}(x,y^*)| \leq L_1|y-y^*| \tag{4.6.7}$$

and

$$|f^{(2)}(x,y) - f^{(2)}(x,y^*)| \leq L_2|y-y^*| \tag{4.6.8}$$

for arbitrary points (x,y) and (x,y^*) in R. We have thus established the Lemma (4.1).

The following Lemma will be useful in proving that the increment function $\phi = \phi(x,y;h)$ defined by equation (4.6.2) satisfies the Lipschitz condition. The proof of the Lemma is available in Jones and Jordan (1969) volume 1.

Lemma 4.2

Consider the power series

$$\mathcal{G}(x) = \sum_{i=0}^{\infty} c_i x^i \quad . \tag{4.6.9}$$

If

$$\lim_{i\to\infty} \left|\frac{c_{i+1}}{c_i}\right| \tag{4.6.10}$$

exists and is denoted by $\frac{1}{A}$, then the power series $\mathcal{G}(x)$ given by equation (4.6.9) converges absolutely for $|x| < A$ and diverges for $|x| > A$. A is called the radius of convergence of the power series.

Finally, the following theorem will be required in establishing the stability of the integration formulae given by equation (4.5.2) to (4.5.5).

Theorem 4.1

The increment function $\phi = \phi(x,y;h)$ defined by equation (4.6.2) satisfies the Lipschitz condition.

Proof:

Let (x,y) and (x,y^*) be points in R, and the function $\phi = \phi(x,y;h)$ is given by equation (4.6.2). We wish to exhibit a constant $L^* < \infty$ such that

$$|\phi(x,y;h) - \phi(x,y^*;h)| \leqslant L^*|y-y^*| \quad . \tag{4.6.11}$$

By using equation (4.6.2) in the left hand side of equation (4.6.11), we obtain

$$\begin{aligned} &|\phi(x,y;h) - \phi(x,y^*;h)| \\ &= \Big| [f(x,y)-f(x,y^*)] + h[f^{(1)}(x,y^*)-f^{(1)}(x,y)] \quad \times \\ &\left[\sum_{i=1}^{\infty} (-1)^i \frac{(Nh)^{2i-2}}{(2i)!}\right] + h^2[f^{(2)}(x,y^*)-f^{(2)}(x,y)] \\ &\times \quad \left[\sum_{i=1}^{\infty} (-1)^i \frac{(Nh)^{2i-2}}{(2i+1)!}\right] \Big| \quad . \end{aligned} \tag{4.6.12}$$

Using the triangle inequality in equation (4.6.12) we obtain the following relationship

$$|\phi(x,y;h) - \phi(x,y^*;h)| \leq$$

$$|f(x,y)-f(x,y^*)| + h|f^{(1)}(x,y^*)-f^{(1)}(x,y)| \left|\sum_{i=1}^{\infty}(-1)^i \frac{(Nh)^{2i-2}}{(2i)!}\right|$$

$$+ h^2|f^{(2)}(x,y^*) - f^{(2)}(x,y)| \left|\sum_{i=1}^{\infty}(-1)^i \frac{(Nh)^{2i-2}}{(2i+1)!}\right| \quad . \tag{4.6.13}$$

We have obtained the Lipschitz constants L_*, L_1 and L_2 respectively for the functions $f(x,y), f^{(1)}(x,y)$ and $f^{(2)}(x,y)$ from Lemma (4.1).

Let R_1 be the radius of convergence of the power series

$$W_1(x) = \sum_{i=1}^{\infty}(-1)^i \frac{(Nh)^{2i-2}}{(2i)!} \tag{4.6.14}$$

and R_2, the radius of convergence of the power series

$$W_2(x) = \sum_{i=1}^{\infty}(-1)^i \frac{(Nh)^{2i-2}}{(2i+1)!} \quad . \tag{4.6.15}$$

By applying Lemma (4.2) to the two power series $W_1(x)$ and $W_2(x)$ as defined by equations (4.6.14) and (4.6.15), we obtain $R_1 = \infty$ and $R_2 = \infty$. Hence if the mesh-size h and the first parameter N satisfy the condition:

$$|Nh| < \infty \quad , \tag{4.6.16}$$

then the two power series $W_1(x)$ and $W_2(x)$ both converge absolutely to $k_1 < \infty$ and $k_2 < \infty$ respectively.

We now have the following result from equation (4.6.13):

$$|\phi(x,y;h) - \phi(x,y^*;h)| \leq$$

$$(L_* + L_1 k_1 h + L_2 k_2 h^2)\,|y-y^*| \quad , \tag{4.6.17}$$

If we set

$$L^* = L_* + L_1 k_1 h + L_2 k_2 h^2 < \infty \tag{4.6.18}$$

then equation (4.6.17) yields

$$|\phi(x,y;h) - \phi(x,y;h)| < L^* \, |y-y^*| \quad .$$

We have thus proved that the increment function to the integration formula (4.5.2) and defined by equation (4.6.2) satisfies a Lipschitz condition. We are now well equiped to establish the stability of formula (4.5.2). We now present the following theorem:

Theorem 4.2

If the increment function $\phi = \phi(x,y;h)$ satisfies the Lipschitz condition, then the one step scheme defined by equations (4.6.2) and (4.6.3) is stable.

Proof:

Let $y(x)$ and $y^*(x)$ be two different numerical solutions of the initial value problem (4.2.1) with initial conditions:

$$y(a) = \eta; \text{ and } y^*(a) = \eta^* \quad . \tag{4.6.18}$$

Then by applying equation (4.6.3), $y(x)$ and $y^*(x)$ satisfy respectively the following relations:

$$y_t = y_{t-1} + h\phi(x_{t-1},y_{t-1};h) \tag{4.6.19}$$

and

$$y_t^* = y_{t-1}^* + \phi(x_{t-1},y_{t-1}^*;h) \quad . \tag{4.6.20}$$

Subtracting equation (4.6.20) from equation (4.6.19), we get

$$y_t-y_t^* = y_{t-1} - y_{t-1}^* + h\left[\phi(x_{t-1},y_{t-1};h)-\phi(x_{t-1},y_{t-1}^*;h)\right] \quad . \tag{4.6.21}$$

By taking the norms of both sides of equation (4.6.21) we get

$$|y_t-y_t^*| = \left|(y_{t-1}-y_{t-1}^*)+h\left[\phi(x_{t-1},y_{t-1};h)-\phi(x_{t-1},y_{t-1}^*;h)\right]\right|$$

and applying the triangle inequality in the last equation, we obtain the relation;

$$|y_t-y_t^*| \leq |y_{t-1}-y_{t-1}^*| + h|\phi(x_{t-1},y_{t-1};h)-\phi(x_{t-1},y_{t-1}^*;h)| . \tag{4.6.22}$$

Since by theorem (4.1) the increment function $\phi = \phi(x,y;h)$ satisfies a Lipschitz condition in y, there exists a constant $L^*<\infty$ such that

$$|\phi(x_{t-1},y_{t-1};h) - \phi(x_{t-1},y^*_{t-1};h)| \leq L^*|y_{t-1}-y^*_{t-1}| . \qquad (4.6.23)$$

Using equation (4.6.23) in equation (4.6.22) gives the following relationship:

$$|y_t-y^*_t| \leq (1+hL^*)\ |y_{t-1}-y^*_{t-1}| \qquad (4.6.24)$$

By a similar argument to the above, the relation,

$$|y_{t-1}-y^*_{t-1}| \leq (1+hL^*)|y_{t-2}-y^*_{t-2}| \quad \text{holds.} \qquad (4.6.25)$$

This process can be repeated t-1 times to obtain

$$|y_2-y^*_2| \leq (1+hL^*)\ |y_1-y^*_1|$$

and finally

$$|y_1-y^*_1| \leq (1+hL^*)|\eta-\eta^*| .$$

Hence, by repeated backward substitution we obtain the following relationship from equation (4.6.2),

$$|y_t-y^*_t| \leq (1+hL^*)^t\ |\eta-\eta^*| . \qquad (4.6.26)$$

By setting

$$k = (1+hL^*)^t < \infty$$

equation (4.6.26) gives

$$|y_t-y^*_t| \leq k\ |\eta-\eta^*| \qquad (4.6.27)$$

Equation (4.6.27) establishes the stability of the one step integration formula (4.5.2) which has been proved to be of order four.

By using similar arguments for the higher order schemes given by equations (4.5.3) to (4.5.5) we can also establish their stability.

4.7 CONVERGENCE

We shall discuss briefly in this section, the convergence and consistency properties of the one-step schemes given by equations (4.5.2) to (4.5.5).

With the definitions (2.3.2) and (2.3.3), we now use a theorem given by Henrici (1962):

Let the increment function $\phi = \phi(x,y;h)$ of a one step scheme be continuous in x,y and h for $a \leq x \leq b$, $0 \leq h \leq h_0$ and for all y in $-\infty < y < \infty$ and if it satisfies a Lipschitz condition in the same region, a necessary and sufficient condition for convergence of the one-step scheme is that it is consistent.

We now apply this theorem to the fourth order one step scheme given by equations (4.6.2) and (4.6.3). We have established in Theorem (4.1) that the increment function $\phi = \phi(x,y;h)$ as defined by equations (4.6.2) satisfies the Lipschitz condition with respect to y. $\phi = \phi(x,y;h)$ is also continuous in x,y and h and satisfies the consistency criteria given by the definition (2.3.2). Hence the fourth order one step scheme given by equation (4.5.2) is consistent. By the above theorem, we can assert that the same scheme is convergent. An identical argument can be made for the higher order integration schemes given by equations (4.5.3) to (4.5.5).

We shall discuss in the next section, the alternative interpolating function in the event of the failure of the interpolating function (4.2.6).

4.8 ALTERNATIVE INTERPOLANT

In the eventuality that the interpolating function given by equation (4.2.6) fails as a result of the parameter N_t vanishing or becoming infinite, indeterminate or complex and if varying the degree of the polynomial part of the interpolant is of no avail, we use the alternative interpolant given by:

$$F_t(x) = \sum_{r=0}^{L} a_r x_t^r + b_t \sinh(N_t x_t + A_t) \quad . \tag{4.8.1}$$

By following the same procedure as outlined in sections (4.3) to (4.5), for the interpolating function (4.2.6) we obtained the following results:

(a) The parameters N_t and A_t are now given as follows:

$$N_t = \left[\frac{f^{(L+2)}(x_t,y_t)}{f^{(L)}(x_t,y_t)}\right]^{\frac{1}{2}} \tag{4.8.2}$$

and

$$A_t = \coth^{-1}\left(\frac{f^{(L+1)}(x_t,y_t)}{N_t f^{(L)}(x_t,y_t)}\right) - N_t x_t \tag{4.8.3}$$

when the degree L of the polynomial part of equation (4.8.1) is odd or

$$A_t = \tanh^{-1}\left|\frac{f^{(L+1)}(x_t,y_t)}{N_t f^{(L)}(x_t,y_t)}\right| - N_t x_t \tag{4.8.4}$$

when L is even.

(b) The final integration formulae are given as follows:

(i) <u>For L=1</u>

$$y_{t+1} = y_t + hf(x_t,y_t) + f^{(1)}(x_t,y_t)\left[\cosh(N_t h)-1\right] + f^{(2)}(x_t,y_t)\left[\sinh(N_t h) - N_t h\right] \tag{4.8.5}$$

(ii) For L=2,

$$y_{t+1} = y_t + \sum_{r=1}^{L} \frac{h^r}{r!} f^{(r-1)}(x_t,y_t)$$

$$+ \frac{f^{(2)}(x_t,y_t)}{N_t^3} \left[\sinh(N_t h) - N_t h\right]$$

$$+ \frac{f^{(3)}(x_t,y_t)}{N_t^4} \left\{ \cosh(N_t h) - \left[1 + \frac{(N_t h)}{2!}\right]^2 \right\} \qquad (4.8.6)$$

(iii) For L=3

$$y_{t+1} = y_t + \sum_{r=1}^{L} \frac{h^r}{r!} f^{(r-1)}(x_t,y_t)$$

$$+ \frac{f^{(3)}(x_t,y_t)}{N_t^4} \left\{ \cosh(N_t h) - \left[1 + \frac{(N_t h)^2}{2!}\right] \right\}$$

$$+ \frac{f^{(4)}(x_t,y_t)}{N_t^5} \left\{ \sinh(N_t h) - \left[N_t h + \frac{(N_t h)^3}{3!}\right] \right\} \qquad (4.8.7)$$

and finally

(iv) For L=4

$$y_{t+1} = y_t + \sum_{r=1}^{L} \frac{h^r}{r!} f^{(r-1)}(x_t,y_t)$$

$$+ \frac{f^{(4)}(x_t,y_t)}{N_t^5} \left\{ \sinh(N_t h) - \left[N_t h + \frac{(N_t h)^3}{3!}\right] \right\}$$

$$+ \frac{f^{(5)}(x_t,y_t)}{N_t^6} \left\{ \cosh(N_t h) - \left[1 + \frac{(N_t h)^2}{2!} + \frac{(N_t h)^4}{4!}\right] \right\}$$

(4.8.8)

(c) The truncation errors for the integration schemes of various orders are obtained by using the following expansions:

$$\cosh(N_t h) = \sum_{i=0}^{\infty} \frac{(N_t h)^{2i}}{(2i)!} \qquad (4.8.9)$$

and

$$\sinh(N_t h) = \sum_{i=0}^{\infty} \frac{(N_t h)^{2i+1}}{(2i+1)!} \qquad (4.8.10)$$

instead of the sine and cosine expansions used in section 4.

The truncation errors are now as follows:

(i) For L=1

$$T_{t+1} = \sum_{s=L+2}^{\infty} \frac{h^{2s}}{(2s)!} \left[f^{(2s-1)}(x_t,y_t) - N_t^{2s-L-1} f^{(L)}(x_t,y_t)\right] + \sum_{s=L+1}^{\infty} \frac{h^{2s+1}}{(2s+1)!} \left[f^{(2s)}(x_t,y_t) - N_t^{2s-L-1} f^{(L+1)}(x_t,y_t)\right] \qquad (4.8.11)$$

(ii) For L=2

$$T_{t+1} = \sum_{s=L+1}^{\infty} \frac{h^{2s+1}}{(2s)!} \left[f^{(2s)}(x_t,y_t) - N_t^{2s-L} f^{(L)}(x_t,y_t)\right] + \sum_{s=L+1}^{\infty} \frac{h^{2s}}{(2s+1)!} \left[f^{(2s-1)}(x_t,y_t) - N_t^{2s-L-2} f^{(L+1)}(x_t,y_t)\right]$$

(4.8.12)

(iii) For L=3

$$T_{t+1} = \sum_{s=L+1}^{\infty} \frac{h^{2s}}{(2s)!} \left[f^{(2s-1)}(x_t,y_t) - N_t^{2s-L-1} f^{(L)}(x_t,y_t)\right] + \sum_{s=L}^{\infty} \frac{h^{2s+1}}{(2s+1)!} \left[f^{(2s)}(x_t,y_t) - N_t^{2s-L-1} f^{(L+1)}(x_t,y_t)\right],$$

and finally (4.8.13)

(iv) For L=4

$$T_{t+1} = \sum_{s=L}^{\infty} \frac{h^{2s+1}}{(2s+1)!} \left[f^{(2s)}(x_t,y_t) - N_t^{2s-L} f^{(L)}(x_t,y_t)\right] + \sum_{s=L}^{\infty} \frac{h^{2s}}{(2s)!} \left[f^{(2s-1)}(x_t,y_t) - N_t^{2s-L-2} f^{(L+1)}(x_t,y_t)\right].$$

(4.8.14)

We observed from equations (4.8.11) to (4.8.14) that the degree L of the polynomial part of the interpolating function (4.8.1) and the order p of the resultant integration formulae satisfy the relation given by equation (4.5.7).

(d) We shall now discuss briefly, the stability and convergence charactersitics of the one step integration formulae given in equations (4.8.5) to (4.8.8). By using the equations (4.8.9) and (4.8.10) in the fourth order integration formula (4.8.5), we obtain

$$y_{t+1} = y_t + h\Big[f(x_t,y_t)+hf^{(1)}(x_t,y_t)\cdot \sum_{i=1}^{\infty}\frac{(N_t h)^{2i-2}}{(2i)!}$$

$$+ h^2 f^{(2)}(x_t,y_t)\ \Big(\sum_{i=1}^{\infty}\frac{(N_t h)^{2i-2}}{(2i+1)!}\Big)\Big] \quad . \tag{4.8.15}$$

We now define the increment function $\psi = \psi(x,y;h)$ as:

$$\psi(x,y;h) = f(x,y) + hf^{(1)}(x,y)\ \Big(\sum_{i=1}^{\infty}\frac{(Nh)^{2i-2}}{(2i)!}\Big)$$

$$+ h^2 f^{(2)}(x,y)\ \Big(\sum_{i=1}^{\infty}\frac{(Nh)^{2i-2}}{(2i+1)!}\Big) \quad . \tag{4.8.16}$$

Using equation (4.8.16) in (4.8.15), the fourth order scheme given by equation (4.8.5) can be expressed as

$$y_{t+1} = y_t + h\psi(x_t,y_t;h) \quad . \tag{4.8.17}$$

The increment function $\psi = \psi(x,y;h)$ given by equation (4.8.16) is continuous in x,y and h and satisfies the Lipschitz condition with respect to y. Hence, by making similar arguments for $\psi(x,y;h)$ as those made for $\phi(x,y;h)$ in sections (4.6) and (4.7), we can establish that the integration formula defined by equation (4.8.5) is stable and convergent. Identical results hold for the higher order formulae defined by equations (4.8.6) to (4.8.8).

Some possible causes of the failure of the integration schemes are:

(a) the parameter N_t vanishing or becoming infinite, indeterminate or complex.

(b) the argument z of arc tanh does not lie in the range

$$-1<z<1$$

(c) the argument of arc coth lies outside the range $z<-1$ and $z>1$.

In the event that any of the conditions (a),(b) or (c) does occur, we vary the degree of the polynomial part of the interpolant (4.8.1). If this does not remedy the situation, we switch to the interpolating function (4.2.6).

The failure (b) and (c) rarely occur. Cases of failure (a) occurring are treated in the numerical applications discussed in the next section.

4.9 Applications and Numerical Results

Example (4.9.1)

We first consider the scalar initial value problem

$$y' = -(1-y^2)^{\frac{1}{2}} \quad , \; y(0)=1 \qquad (4.9.1)$$

over the range $0 \leqslant x \leqslant \pi$.

The theoretical solution of problem (4.9.1) in the specified range is $y(x)=\cos x$. The numerical solution was obtained with uniform mesh-size $h=\frac{\pi}{10}$ using schemes of orders 4,5,6 and 7. For the integration schemes of orders 5 and 7, the parameter N_t was indeterminate at $x=0$. Hence, in each case, there was a switch to the integration scheme of order 6 as the specified maximum available order is 7. The parameter N_t was constant with unit value throughout the interval of integration. The parameter A_t has constant value $+\frac{\pi}{2}$ in the range $0 \leqslant x \leqslant \frac{\pi}{2}$ and constant value $-\frac{\pi}{2}$ in the range $\frac{\pi}{2} \leqslant x \leqslant \pi$. We can observe from Table 4.9.1 that the numerical results obtained by the fourth order integration scheme are correct to 10 decimal places.

TABLE 4.9.1

Fourth Order Schemes

t	h	x_t	NUMERICAL y_t SOLUTION	MIXED ERROR FOR ORDER 4 $10^{10}\ T_{t+1}$	MIXED ERROR FOR ORDER 6 $10^{10}\ T_{t+1}$
0	0.31415926	0.00000000	1.00000000	0.00000000	0.00000000
1	0.31475926	0.31415926	0.95105652	0.00000000	0.07458479
2	0.31415926	0.62831852	0.80901700	0.20110252	0.04022050
3	0.31415926	0.94247778	0.58778527	0.50407026	0.04582456
4	0.31415926	1.25663704	0.30901701	0.80595885	0.08337505
5	0.31415926	1.57079630	0.00000003	1.39152460	0.36497019
6	0.31415926	1.88495556	-0.30901696	0.69479214	0.05558337
7	0.31415926	2.19911482	-0.58778522	0.59571942	0.04582457
8	0.31415926	2.51327408	-0.80901697	0.32176404	0.00000000
9	0.31415926	2.82743334	-0.95105650	0.03729239	0.07458479
10	0.31415926	3.14159265	-1.00000000	0.00000000	0.03637978

Example 4.9.2

We also consider the example given by Amdursky and Ziv(1974). The system is given by

$$\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{\beta^2}{x^2} & -\frac{1}{x} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \tag{4.9.2}$$

where β is a real constant. The general solution of problem (4.9.2) is

$$y_1(x) = A\sin(\beta\log x)+B\cos(\beta\log x)$$

$$y_2(x) = \beta\left[A\cos(\beta\log x)-B\sin(\beta\log x)\right]/x$$

We obtained the numerical solution of problem (4.9.2) in the interval $e^2 \leq x \leq 9$, where $e=2.7182818$ with a uniform step size $h=0.1$. The following numerical values are assigned to the real numbers A, B and β:

$$A=1, \quad B=1 \text{ and } \quad \beta=1 \quad ;$$

thus giving the initial conditions

$$y_1(e^2) = 1 \quad \text{and}$$

$$y_2(e^2) = \frac{\pi}{e^2} \quad .$$

Details of the numerical results are given in tables ($4.9.2^A$) and ($4.9.2^B$) .

TABLE 4.9.2A

t	X_t	$N_t^{(1)}$	$A_t^{(1)}$	$Y_t^{(1)}$	MIXED ERROR $10^7 \times T_{t+1}^{(1)}$
0	7.3890561	0.4686608	-1.7841529	1.00000000	0.00000000
1	7.4890561	0.4462486	-1.6109432	1.0413275	0.0524669
2	7.5890561	0.4246877	-1.4393799	1.0802870	0.0565208
3	7.6890561	0.4038547	-1.2686623	1.1168977	0.0526561
4	7.7890561	0.3836360	-1.0980135	1.1511833	0.0434288
5	7.8890561	0.3639247	-0.9266579	1.1831711	0.0289282
6	7.9890561	0.3446179	-0.7537964	1.2128918	0.0124286
7	8.0890561	0.3256132	-0.5785795	1.2403792	0.0073397
8	8.1890561	0.3068057	-0.4000722	1.2656697	0.0288383
9	8.2890561	0.2880840	-0.2172096	1.2888020	0.0514988
10	8.3890561	0.2693245	-0.0287342	1.3098170	0.0759153
11	8.4890561	0.2503841	0.1668964	1.3287572	0.1015428
12	8.5890561	0.2310889	0.3716535	1.3456666	0.1274249
13	8.6890561	0.2112150	0.5881757	1.3605905	0.1541131
14	8.7890561	0.1904553	0.8201953	1.3735754	0.1809199
15	8.8990561	0.1683542	1.0733758	1.3846685	0.2083318
16	8.9890561	0.1441603	1.3571882	1.3939178	0.2364615
17	9.0000000	-	-	1.4013717	0.2645724

TABLE 4.9.2[B]

t	X_t	$N_t^{(2)}$	$A_t^{(2)}$	$Y_t^{(2)}$	MIXED ERROR $10^7\ xT_{t+1}^{(2)}$
0	7.3890561	2.1071631	-15.1163220	0.4251683	0.0000000
1	7.4890561	1.7079582	-12.2370060	0.4014065	0.1884658
2	7.5890561	1.4630608	-10.4633550	0.3778151	0.2946419
3	7.6890561	1.2921509	-9.2188272	0.3544389	0.3733226
4	7.7890561	1.1634728	-8.2755737	0.3313180	0.4358793
5	7.8890561	1.0616019	-7.5228248	0.3084884	0.4864398
6	7.9890561	0.9780172	-6.8995709	0.2859818	0.5298624
7	8.0890561	0.9075732	-6.3688757	0.2638267	0.5660654
8	8.1890561	0.8469524	-5.9069497	0.2420478	0.5981931
9	8.2890561	0.7939055	-5.4976599	0.2206671	0.6260311
10	8.3890561	0.7468446	-5.1296142	0.1997035	0.6496155
11	8.4890561	0.7046117	-4.7944973	0.1791732	0.6704590
12	8.5890561	0.6663388	-4.4860675	0.1590902	0.6894045
13	8.6890561	0.6313598	-4.1995259	0.1394661	0.7054440
14	8.7890561	0.5991532	-3.9311043	0.1203106	0.7190403
15	8.8890561	0.5693035	-3.6777870	0.1016315	0.7309764
16	8.9890561	0.5415739	-3.4371180	0.0834346	0.7407268
17	9.0000000	-	-	0.0657246	0.7485812

Example 4.9.3

We also consider the scalar initial value problem

$$y' = -2xy + 4x, \; y(0)=3 \tag{4.9.3}$$

in the interval $0 \leq x \leq 1.025$. The theoretical solution to problem (4.9.3) is $y(x)=e^{-x^2} + 2$.

The numerical solution to problem (4.9.3) was obtained with an initial stepsize $h=0.1$ and specified tolerance $e=10^{-8}$. As the solution to the problem is not oscillatory, there was a switch to the hyperbolic interpolant in the range $0.5 \leq x \leq 0.7125$. The non-oscillatory nature of the problem also accounts for the small stepsize required to obtain the desired accuracy.

Details of the numerical results are given in table (4.9.3).

TABLE 4.9.3

INDEX	h	X_t	N_t	A_t	Y_t	$10^8 x T_{t+1}$
1	0.10000	0.00000	2.4433378	1.05712060	3.0000000	0.00000
1	0.05000	0.10000	2.3699187	1.5891165	2.9900498	0.20715
1	0.02500	0.20000	2.2326413	1.6477103	2.9607895	0.56800
1	0.02500	0.30000	1.9678116	1.7972221	2.9139312	0.63949
1	0.02500	0.40000	1.3446956	2.2070509	2.8521438	0.74041
1	0.02500	0.50000	2.2300382	-1.5702748	2.7788008	0.87724
2	0.01250	0.60625	4.0541435	-2.8667117	2.6924363	0.92930
2	0.00625	0.71250	4.6610851	-3.2860414	2.6019047	0.91063
1	0.02500	0.82500	3.6347782	-2.5345045	2.5063004	0.32123
1	0.02500	0.92500	3.1622777	-2.1554240	2.4250175	0.54808
1	0.02500	1.02500	-	-	2.3497191	0.63686

INDEX = 1 Polynomial and Trigonometric Interpolant

INDEX = 2 Polynomial and Hyperbolic Interpolant

Example (4.9.4)

We finally consider the Van-der-Pol oscillator in the form

$$\begin{aligned} y_1' &= y_2 \ , \ y_1(0) = 0 \\ y_2' &= 0.01(1-y_1^2)y_2-y_1, \ y_2(0)=1 \end{aligned} \qquad (4.9.4)$$

over the range $0 \leqslant x \leqslant 6$.

The numerical solution to the initial value problem (4.9.4) was obtained using the following integration schemes:

(a) the fourth order one-step scheme as given by equation (4.5.2)

(b) the Krogh's variable order Adams scheme(The Numerical Algorithm Group's version).

(c) the Gragg-Bulirsch-Stoer (G-B-S) rational extrapolation scheme.

All the numerical integration subroutines are written in FORTRAN IV for the ICL 1904A computer with single precision arithmetic.

A uniform mesh size of h=0.0375 was specified in the three schemes. The new integration algorithm varied its order at the mesh points x=0, x=1.5 and x=4.6875. Whilst the new algorithm required 171 function evaluations, Krogh's scheme required 453 function evaluations and the G-B-S scheme required 37,020 function evaluations. Also, the total machine time required by the new scheme was 63 seconds whilst Krogh's scheme required 69 seconds and the G-B-S scheme required 91 seconds. The running cost for the new scheme under the accounting system operational on the Loughborough University machine was 38 pence whilst the running cost for Krogh's scheme was 39 pence and 49 pence for the G-B-S scheme.

The details of the numerical results are given in table (4.9.4).

TABLE 4.9.4

X	FOURTH ORDER ONE STEP SCHEME Y_1	FOURTH ORDER ONE STEP SCHEME Y_2	KROGH VARIABLE ORDER Y_1	KROGH VARIABLE ORDER Y_2	GRAGG-BULIRSCH-STOER Y_1	GRAGG-BULIRSCH-STOER Y_2
0.00000000	0.00000000	1.00000000	0.00000000	1.00000000	0.00000000	1.00000000
0.30000000	0.29595737	0.95816542	0.29595737	0.95816542	0.29595738	0.95816542
0.60000000	0.56624448	0.83005702	0.56624448	0.83005702	0.56624449	0.83005701
0.90000000	0.78645340	0.62681152	0.73645340	0.62681152	0.78645341	0.62681151
1.20000000	0.93663469	0.36677933	0.93663469	0.36677933	0.93663469	0.36677931
1.50000000	1.00320104	0.07364129	1.00320104	0.07364129	1.00320105	0.07364127
1.80000000	0.98015691	-0.22611779	0.98015691	-0.22611777	0.98015691	-0.22611779
2.10000000	0.86954204	-0.50583247	0.86954204	-0.50583245	0.86954203	-0.50583247
2.40000000	0.68113086	-0.74094526	0.68113087	-0.74094524	0.68113085	-0.74094526
2.70000000	0.43151588	-0.91082896	0.43141490	-0.91082894	0.43151587	-0.91082896
3.00000000	0.14270079	-1.00026329	0.14270081	-1.00026329	0.14270077	-1.00026330
3.30000000	-0.015971789	-1.00071514	-0.15971786	-1.00071515	-0.15971790	-1.00071514
3.60000000	-0.44872183	-0.91138069	-0.44872180	-0.91138071	-0.44872184	-0.91138069
3.90000000	-0.69828521	-0.73970197	-0.69828519	-0.73970199	-0.69828522	-0.73970195
4.20000000	-0.88581762	-0.50098678	-0.88581760	-0.50098681	-0.88581763	-0.50098676
4.50000000	-0.99433194	-0.21695595	-0.99433193	-0.21695598	-0.99433195	-0.21695592
4.80000000	-1.01403600	0.08658086	-1.01403600	+0.08658083	-1.01403600	0.08658089
5.10000000	-0.94315793	0.38241170	-0.94315794	0.38241166	-0.94315792	0.38241172
5.40000000	-0.78798032	0.64443656	-0.78798033	0.64443653	-0.78798029	0.64443659
5.70000000	-0.56218592	0.84972276	-0.56218595	0.84972273	-0.56218589	0.84972277
6.00000000	-0.28565523	0.98012923	-0.28565527	0.98012921	-0.28565519	0.98012924

4.10. CONCLUSION

From example such as (4.9.1), we observed that the numerical integration procedure developed in this chapter will allow relatively large integration step-sizes and still maintains a high degree of accuracy particularly when the theoretical solution contains sine and cosine functions.

The fact that the proposed one-step scheme uses higher order derivatives of the given differential equations enables us to obtain a solution to problem (4.9.1) at x=0 where the initial value problem has no unique solution as it fails to satisfy the hypothesis of theorem (1.1).

The main disadvantage of the proposed scheme is the requirement to obtain higher order derivatives of f(x,y) analytically. In some problems these are readily obtainable, all the same, we shall remedy this situation in the next Chapter.

CHAPTER V

AN EXPLICIT MULTISTEP NUMERICAL INTEGRATION SCHEME FOR SOLVING SYSTEMS OF ORDINARY DIFFERENTIAL EQUATIONS WITH OSCILLATORY SOLUTIONS

5.1 INTRODUCTION

In Lambert and Shaw (1965) and Shaw (1967), some linear multistep integration formulae were formulated to solve initial value problems of the form

$$y' = f(x,y),\ y(a) = \eta\ . \tag{5.1.1}$$

These numerical integration schemes are based on the representation of the solution to the initial value problem (5.1.1) by non-polynomial interpolants as given by equation (2.6.1). The resultant integration formulae are particularly well suited to solving initial value problems whose solutions contain singularities.

In Chapter IV, we proposed a stable and convergent one-step integration scheme for solving initial value problems of the form (5.1.1). The numerical integration schemes are based on a local representation of the solution on every subinterval $I_t = x_t \leq x \leq x_{t+1}$, $t=0,1,\ldots$ by either the interpolating function,

$$F_t(x) = \sum_{r=0}^{L} a_r x^r + b_t \sin(N_t x + A_t) \tag{5.1.2}$$

or

$$F_t(x) = \sum_{r=0}^{L} a_r x^r + b_t \sinh(N_t x + A_t) \tag{5.1.3}$$

where L is a non-negative integer; b_t and $\{a_r, r=0,1,\ldots,L\}$ are real undetermined coefficients and N_t, A_t are real parameters which are evaluated at each step of the integration procedure. The determination of the parameters N_t and A_t however requires the analytic evaluation of higher derivatives of $f=f(x,y)$ given by equation (5.1.1). As this could be very cumbersome particularly if $f(x,y)$ is a very complicated expression, we shall develop in this chapter, a linear multistep scheme which circumvents the analytic determination of the higher derivatives of $f(x,y)$. However, we now have to solve a pair of trigonometric (or hyperbolic) equations for the parameters N_t and A_t. A device is also introduced for obtaining good initial estimates for these parameters as the effectiveness of the Newton iteration method is critically dependent on the choice of these estimates. The starting values for the multistep formulae are obtained from the version of the Gragg-Bulirsch-Stoer rational extrapolation scheme discussed in Chapter III. The proposed scheme is convergent and zero-stable.

5.2 INTERPOLATING FUNCTIONS AND DETERMINATION OF THE PARAMETERS N_T AND A_T

We shall denote by k the stepnumber of the multistep integration formulae and any necessary additional starting values (i.e. $y_1, y_2, \ldots, y_{k-1}$) are obtained with the variable order Gragg-Bulirsch-Stoer algorithm discussed in Chapter III.

Let us assume that the numerical solutions $y_t, y_{t+1}, \ldots, y_{t+k-1}$ have been obtained at the points $x_t, x_{t+1}, \ldots x_{t+k-1}$ respectively. We now wish to obtain the numerical solution y_{t+k} at the point $x = x_{t+k}$.

Let

$$I^* = \bigcup_{i=0}^{k-1} I_{t+i} \quad \text{for } 0 \leq t \leq N-k, \tag{5.2.1}$$

be the union of the subintervals $I_t, I_{t+1}, \ldots, I_{t+k-1}$ defined by equations (4.2.3) and (4.2.4).

Over the interval I*, the solution to each equation in the initial value problem is represented by the interpolating function (5.1.2).

We shall denote by f_{t+j}, the value of the function f(x,y) at the point $x = x_{t+j}, y = y_{t+j}$. In an attempt to eliminate the undetermined coefficients in the interpolating function (5.1.2), the following constraints are imposed on the interpolant (5.1.2):

(a) the interpolating function should pass through the points $\{(x_{t+j}, y_{t+j}), j=0,1,\ldots,k\}$

i.e.

$$F_t(x_{t+j}) = y_{t+j}, \; j=0,1,\ldots,k \tag{5.2.2}$$

(b) the first derivative of the interpolating function must satisfy the differential equation (5.1.1) at those points specified in condition (a). i.e.

$$\left.\frac{dF_t(x)}{dx}\right|_{\substack{x=x_{t+j}\\ y=y_{t+j}}} = f_{t+j},\ j=0,1,\ldots,k-1\,. \qquad (5.2.3)$$

Equations (5.2.2) and (5.2.3) respectively imply that the relations

$$\sum_{i=0}^{L} a_i x_{t+j}^{i} + b_t \sin(N_t x_{t+j}+A_t) = y_{t+j},\ j=0,1,\ldots,k \qquad (5.2.4)$$

and

$$\sum_{i=0}^{L} i a_i x_{t+j}^{i-1} + b_t N_t \cos(N_t x_{t+j}+A_t) = f_{t+j},\ j=0,1,\ldots,k-1 \qquad (5.2.5)$$

hold.

The forward difference operator Δ discussed in Chapter II has the following relationship with the derivative $f_i=f(x_i,y_i)$ of y at $x=x_i$:

$$\Delta y_i \approx hf_i \quad . \qquad (5.2.6)$$

As the polynomial part of the equation (5.2.5) is of degree at most L-1; theorem (2.1) implies that the application of the operator Δ^L to both sides of equation (5.2.5) will annihilate the polynomial part. This gives

$$b_t N_t \Delta^L \cos(N_t x_{t+j}+A_t) = \Delta^L f_{t+j}\ ,$$

i.e.

$$b_t = \frac{\Delta^L f_{t+j}}{N_t \Delta^L \cos(N_t x_{t+j}+A_t)}\ ,\ j=0,1,\ldots,k-1\ . \qquad (5.2.7)$$

In particular by setting j=0,1,2 in equation (5.2.7), the undetermined coefficient b_t can be obtained as either

$$b_t = \frac{\Delta^L f_t}{N_t \cdot \Delta^L \cos(N_t x_t + A_t)}$$

or

$$b_t = \frac{\Delta^L f_{t+1}}{N_t \cdot \Delta^L \cos(N_t x_{t+1} + A_t)}$$

or

$$b_t = \frac{\Delta^L f_{t+2}}{N_t \cdot \Delta^L \cos(N_t x_{t+2} + A_t)} \quad \cdot \qquad (5.2.8)$$

Hence, the following equations are obtainable from equation (5.2.8):

$$R_1(N_t, A_t) = \Delta^L \cos(N_t x_t + A_t) \;.\; \Delta^L f_{t+1} - \Delta^L \cos(N_t x_{t+1} + A_t) . \Delta^L f_t = 0, \qquad (5.2.9)$$

$$R_2(N_t, A_t) = \Delta^L \cos(N_t x_{t+1} + A_t) . \Delta^L f_{t+2} - \Delta^L \cos(N_t x_{t+2} + A_t) \Delta^L f_{t+1} = 0, \qquad (5.2.10)$$

and finally,

$$R_3(N_t, A_t) = \Delta^L \cos(N_t x_{t+2} + A_t) \Delta^L f_t - \Delta^L \cos(N_t x_t + A_t) \Delta^L f_{t+2} = 0 \;\cdot \qquad (5.2.11)$$

Any two pairs of the equations (5.2.9) to (5.2.11) can be solved for the parameters N_t and A_t.

We now give a detailed discussion of the determination of the parameters N_t and A_t by using equations (5.2.9) and (5.2.10) for the case when the polynomial part of the interpolant (5.1.2) is of degree one (i.e. L=1). We adopt the Newton iteration scheme.

Simplifying equations (5.2.9) we get

$$R_1(N_t,A_t) = (f_{t+2}-f_{t+1})\left[\cos(N_t x_{t+1}+A_t) - \cos(N_t x_t+A_t)\right] - (f_{t+1}-f_t)\left[\cos(N_t x_{t+2}+A_t)-\cos(N_t x_{t+1}+A_t)\right]=0 , \tag{5.2.12}$$

and similarly from equation (5.2.10), we have

$$R_2(N_t,A_t) = (f_{t+3}-f_{t+2})\left[\cos(N_t x_{t+2}+A_t)-\cos(N_t x_{t+1}+A_t)\right] - (f_{t+2}-f_{t+1})\left[\cos(N_t x_{t+3}+A_t)-\cos(N_t x_{t+2}+A_t)\right]=0 . \tag{5.2.13}$$

We now apply the Newton Raphson iteration scheme to obtain the roots N_t^* and A_t^* of the trigonometric functions $R_1(N_t,A_t)$ and $R_2(N_t,A_t)$.

The choice of reasonable initial estimates $N_0^{[0]}$ and $A_0^{[0]}$ at t=0 is very important for the convergence of the Newton iteration. Hence, a scheme is proposed to give these initial estimates. The higher order derivatives of the function f=f(x,y) in equations (4.4.13) to (4.4.15) are replaced by their equivalent forward differences. For instance,

$$f^{(s)}(x_0,y_0) \simeq \frac{\Delta^{s+1}y_0}{h^{s+1}} . \tag{5.2.14}$$

By using the relation (2.2.5) in equation (5.2.14), we have

$$f^{(s)}(x_0,y_0) \simeq \frac{1}{h^{s+1}} \sum_{r=0}^{s+1}(-1)^r\binom{s+1}{r}y_{s-r+1} . \tag{5.2.15}$$

The initial estimates of the parameters N_t and A_t are then given by either the equations:

$$N_0^{[0]} = \left[\frac{\Delta^4 y_0}{\Delta^2 y_0}\right]^{\frac{1}{2}} , \tag{5.2.16}$$

and

$$A_0^{[0]} = \cot^{-1}\left[\frac{\Delta^3 y_0}{N_0^{[0]}.\Delta^2 y_0}\right] - N_0^{[0]}.x_0; \tag{5.2.17}$$

or by the following equations:

$$N_0^{[0]} = \left[- \frac{\Delta^5 y_0}{\Delta^3 y_0} \right]^{\frac{1}{2}} , \qquad (5.2.18)$$

and

$$A_0^{[0]} = \tan^{-1} \left[\frac{-\Delta^4 y_0}{N_0^{[0]} \cdot \Delta^3 y_0} \right] - N_0^{[0]} \cdot x_0 \quad . \qquad (5.2.19)$$

These estimates are now improved upon by the Newton iteration method which is discussed below.

At the i^{th} iteration of the Newton Raphson's scheme, the partial derivatives of equations (5.2.12) and (5.2.13) with respect to N_t at $N_t = N_t^{[i]}$ and $A_t = A_t^{[i]}$ are given by

$$R_{1,N_t}(N_t, A_t)\Big|_{\substack{N_t = N_t^{[i]} \\ A_t = A_t^{[i]}}} =$$

$$-(f_{t+2} - f_{t+1}) \left[x_{t+1} \sin(N_t^{[i]} x_{t+1} + A_t^{[i]}) - x_t \sin(N_t^{[i]} x_t + A_t^{[i]}) \right]$$
$$+ (f_{t+1} - f_t) \left[x_{t+2} \sin(N_t^{[i]} x_{t+2} + A_t^{[i]}) - x_{t+1} \sin(N_t^{[i]} x_{t+1} + A_t^{[i]}) \right] , \qquad (5.2.20)$$

$$R_{2,N_t}(N_t, A_t')\Big|_{\substack{N_t = N_t^{[i]} \\ A_t = A_t^{[i]}}} =$$

$$-(f_{t+3} - f_{t+2}) \left[x_{t+2} \sin(N_t^{[i]} x_{t+2} + A_t^{[i]}) - x_{t+1} \sin(N_t^{[i]} x_{t+1} + A_t^{[i]}) \right]$$
$$+ (f_{t+2} - f_{t+1}) \left[x_{t+3} \sin(N_t^{[i]} x_{t+3} + A_t^{[i]}) - x_{t+2} \sin(N_t^{[i]} x_{t+2} + A_t^{[i]}) \right] . \qquad (5.2.21)$$

By also obtaining the partial derivatives of equations (5.2.12) and (5.2.13) with respect to the parameter A_t at $N_t = N_t^{[i]}$ and $A_t = A_t^{[i]}$, we obtain:

$$R_{1,A_t}(N_t,A_t)\Bigg|_{\substack{N_t=N_t^{[i]}\\ A_t=A_t^{[i]}}} =$$

$$-(f_{t+2}-f_{t+1})\left[\sin(N_t^{[i]}x_{t+1}+A_t^{[i]})-\sin(N_t^{[i]}x_t+A_t^{[i]})\right]$$

$$+(f_{t+1}-f_t)\left[\sin(N_t^{[i]}x_{t+2}+A_t^{[i]})-\sin(N_t^{[i]}x_{t+1}+A_t^{[i]})\right], \qquad (5.2.22)$$

and finally,

$$R_{2,A_t}(N_t,A_t)\Bigg|_{\substack{N_t=N_t^{[i]}\\ A_t=A_t^{[i]}}} =$$

$$-(f_{t+3}-f_{t+2})\left[\sin(N_t^{[i]}x_{t+2}+A_t^{[i]})-\sin(N_t^{[i]}x_{t+1}+A_t^{[i]})\right]$$

$$+(f_{t+2}-f_{t+1})\left[\sin(N_t^{[i]}x_{t+3}+A_t^{[i]})-\sin(N_t^{[i]}x_{t+2}+A_t^{[i]})\right]. \qquad (5.2.23)$$

Let J denote the determinant of the Jacobian of the functions $R_1(N_t,A_t)$ and $R_2(N_t,A_t)$, i.e.

$$J = \begin{vmatrix} R_{1,N_t}(N_t^{[i]},A_t^{[i]}) & R_{1,A_t}(N_t^{[i]},A_t^{[i]}) \\ R_{2,N_t}(N_t^{[i]},A_t^{[i]}) & R_{2,A_t}(N_t^{[i]},A_t^{[i]}) \end{vmatrix}.$$

The correction terms $\delta N_i^{[i]}$, $\delta A_t^{[i]}$ for $N_t^{[i]}$ and $A_t^{[i]}$ at the i^{th} iteration of the Newton Raphson's scheme are given by:

$$\begin{bmatrix} \delta N_i^{[i]} \\ \delta A_t^{[i]} \end{bmatrix} = J^{-1} \begin{bmatrix} R_{2,A_t}(N_t^{[i]},A_t^{[i]}), & -R_{2,N_t}(N_t^{[i]},A_t^{[i]}) \\ -R_{1,A_t}(N_t^{[i]},A_t^{[i]}), & R_{1,N_t}(N_t^{[i]},A_t^{[i]}) \end{bmatrix} \times$$

$$\begin{bmatrix} R_1(N_t^{[i]}, A_t^{[i]}) \\ R_2(N_t^{[i]}, A_t^{[i]}) \end{bmatrix} . \tag{5.2.24}$$

The new estimates of the parameters N_t^* and A_t^* are given by

$$N_t^{[i+1]} = N_t^{[i]} + \delta N_t^{[i]}, \tag{5.2.25}$$

and

$$A_t^{[i+1]} = A_t^{[i]} + \delta A_t^{[i]}, \tag{5.2.26}$$

where $\delta N_t^{[i]}$ and $\delta A_t^{[i]}$ are given by equation (5.2.24).

If we define the correction vector $\delta\underline{\alpha}^{[i]}$ by

$$\delta\underline{\alpha}^{[i]} = (N_t^{[i]}, A_t^{[i]})^T, \tag{5.2.27}$$

the Newton iteration is then halted when the condition

$$||\delta\underline{\alpha}^{[i]}|| < \varepsilon_{max} \tag{5.2.28}$$

is satisfied; where ε_{max} is the allowable tolerance.

From practical experience, it may be desirable to set $\varepsilon_{max} \geqslant 10^{-6}$ as it may be impracticable (or time consuming) for the Newton method to obtain accuracy which is less than 10^{-6}.

We denote the terminal values obtained by the Newton method as N_t^* and A_t^* and are given as follows:

$$N_t^* = \lim_{i\to\infty} N_t^{[i]} \tag{5.2.29}$$

and

$$A_t^* = \lim_{i\to\infty} A_t^{[i]} . \tag{5.2.30}$$

In the next section, the parameters N_t^* and A_t^* together with the undetermined coefficient b_t given by equation (5.2.8) will be used to develop a linear multistep scheme to solve the initial value problems of the form (5.1.1).

5.3 Derivation of the Integration Formulae

In this section, we shall eliminate the remaining undetermined coefficients $\{a_r, r=0,1,\ldots,L\}$ in the interpolating function (5.1.2) to obtain a consistent and zero-stable (convergent) linear multistep scheme.

We introduce the function z_{t+i} defined by,

$$z_{t+i} = y_{t+i} - b_t \sin(N_t^* x_{t+i} + A_t^*) \tag{5.3.1}$$

whose derivative z'_{t+i} is then given by

$$z'_{t+i} = f_{t+i} - N_t^* b_t \cos(N_t^* x_{t+i} + A_t^*) \quad . \tag{5.3.2}$$

Equations (5.3.1) and (5.3.2) are then used in equations (5.2.4) and (5.2.5) to yield

$$z_{t+j} = \sum_{i=0}^{L} a_i x_{t+j}^{i} \tag{5.3.3}$$

and

$$z'_{t+j} = \sum_{i=0}^{L} i a_i x_{t+j}^{i-1} \quad . \tag{5.3.4}$$

We now introduce the consistency parameters $\{\alpha_j, \beta_j; j=0,1,\ldots,k\}$ such that α_0, β_0 are not both zero and set $\beta_k=0$ as we are only interested in an explicit formula.

For $j=0,1,\ldots,k$; we multiply equation (5.3.3) by α_j and multiply equation (5.3.4) by $-h\beta_j$ and add columnwise to give:

$$\sum_{j=0}^{k} \alpha_j z_{t+j} - h \cdot \sum_{j=0}^{k} \beta_j z'_{t+j} =$$

$$\sum_{i=0}^{L} a_i \left[\sum_{j=0}^{k} \alpha_j x_{t+j}^{i} - ih \sum_{j=0}^{k} \beta_j x_{t+j}^{i-1} \right] \quad . \tag{5.3.5}$$

As we are only interested in an Adam's type of linear multistep method, we assign the following values to the consistency parameters:

$$\alpha_1 = -1, \quad \alpha_k = +1 \text{ ; and}$$

$$\alpha_j = 0 \quad \text{for } j=0,\ldots,k-1;\ j \neq 1 \qquad (5.3.6)$$

This choice of parameters gives

$$\sum_{j=0}^{k} \alpha_j = 0 \quad , \qquad (5.3.7)$$

which is the first consistency condition for a general linear multistep scheme given by equation (2.4.10).

By applying equations (5.3.6) and (5.3.7) in equation (5.3.5), we have

$$\sum_{j=0}^{k} \alpha_j z_{t+j} - h \cdot \sum_{j=0}^{k-1} \beta_j z'_{t+j}$$

$$= \sum_{i=1}^{L} a_i \Big[\sum_{j=0}^{k} \alpha_j x^i_{t+j} - ih \cdot \sum_{j=0}^{k-1} \beta_j x^{i-1}_{t+j} \Big] . \qquad (5.3.8)$$

By allowing the coefficients of a_i to vanish in equation (5.3.8) (for $i=1,2,\ldots,L$), we obtain

$$\sum_{j=0}^{k} \alpha_j x^i_{t+j} - ih \sum_{j=0}^{k-1} \beta_j x^{i-1}_{t+j} = 0,$$

$$\text{for } i=1,\ldots,L \qquad (5.3.9)$$

There is no loss of generality in assigning the following values

$$x_t = 0 \text{ and } h=1 \qquad (5.3.10)$$

in equation (5.3.9) to obtain

$$\sum_{j=0}^{k} j^i \alpha_j - i \sum_{j=0}^{k-1} j^{i-1} \beta_j = 0 \text{ for } i=1,\ldots,L. \qquad (5.3.11)$$

With a choice of L such that

$$L = k-3 \qquad (5.3.12)$$

equation (5.3.11) will give a set of k-3 equations in the k unknowns $\beta_0, \beta_1, \ldots \beta_{k-1}$ and thus allowing three degrees of freedom.

For the case L=1 and k=4, equation (5.3.11) gives one equation in four unknowns $\beta_0, \beta_1, \beta_2$ and β_3. This equation is the second consistency condition given by equation (2.4.11).

By setting i=2,3 and 4 in equation (5.3.11) we solve for β_1, β_2 and β_3 to give

$$\begin{aligned} \beta_1 &= 1.875 \\ \beta_2 &= -1.125 \\ \beta_3 &= 2.625 \end{aligned} \qquad (5.3.13)$$

The parameter β_0 is then obtained by using equation (5.3.13) in equation (5.3.11) for i=1 to obtain

$$\beta_0 = -0.375 \qquad (5.3.14)$$

The above procedure makes equation (5.3.8) a linear multistep formula. We can associate with (5.3.8) a linear difference operator denoted by $\mathcal{L}$ such that $\mathcal{L}$ operating on an arbitrary function $z(x) \in C^{\infty}[a,b]$ gives the following relationship

$$\mathcal{L}[z(x);h] = \sum_{j=0}^{k} \alpha_j z(x+jh) - h \cdot \sum_{j=0}^{k-1} \beta_j z'(x+jh). \qquad (5.3.15)$$

Replacing z(x+jh) and z'(x+jh) by their respective Taylor's series expansion at the point x in equation (5.3.15), we then obtain

$$\mathcal{L}[z(x);h] = c_0 z(x) + \sum_{i=1}^{\infty} c_i h^i z^{(i)}(x)$$

where the constants c_i, i=0,1,... are given as follows,

$$\begin{aligned} c_0 &= \sum_{j=0}^{k} \alpha_j \\ c_1 &= \sum_{j=1}^{k} j\alpha_j - \sum_{j=0}^{k} \beta_j \\ c_r &= \frac{1}{r!} \sum_{j=1}^{k} j^r \alpha_j - \frac{1}{(r-1)!} \sum_{j=1}^{k} j^{r-1} \beta_j, r=2,3,\ldots \end{aligned} \qquad (5.3.16)$$

By setting $c_r=0$, r=0,1,...4 in equation (5.3.16), we obtain exactly the same set of linear systems from which we solved for $\beta_0, \ldots \beta_3$ to obtain the values in equations (5.3.13) and (5.3.14).

If we take equation (5.3.8) with the coefficient of a_1 set to zero and substituting equation (5.3.1) and (5.3.2), we then have the final integration formula as

$$\sum_{j=0}^{k} \alpha_j y_{t+j} - h \sum_{j=0}^{k-1} \beta_j f_{t+j} =$$

$$\sum_{j=0}^{k} \alpha_j \left[y_{t+j} - b_t \sin(N_t^* x_{t+j} + A_t^*)\right]$$

$$-h \sum \beta_j \left[f_{t+j} - N_t^* b_t \cos(N_t^* x_{t+j} + A_t^*)\right] \qquad (5.3.17)$$

From equation (5.2.8) the undetermined coefficient b_t is now given by

$$b_t = \frac{\Delta f_{t+2}}{N_t^* \cdot \Delta \cos(N_t^* x_{t+2} + A_t^*)}$$

$$= \frac{(f_{t+3} - f_{t+2})}{N_t^* \left[\cos(N_t^* x_{t+3} + A_t^*) - \cos(N_t^* x_{t+2} + A_t^*)\right]} \cdot \qquad (5.3.18)$$

By using equation (5.3.18) in equation (5.3.17) and re-arranging terms, we now have the final integration formula as:

$$y_{t+k} = - \sum_{j=0}^{k-1} \alpha_j y_{t+j} + h \sum_{j=0}^{k-1} \beta_j f_{t+j}$$

$$+ \frac{(f_{t+3} - f_{t+2})}{N_t^* \left[\cos(N_t^* x_{t+3} + A_t^*) - \cos(N_t^* x_{t+2} + A_t^*)\right]} \times$$

$$\left[\sum_{j=0}^{k} \alpha_j \sin(N_t^* x_{t+j} + A_t^*) - N_t^* h \cdot \sum_{j=0}^{k-1} \beta_j \cos(N_t^* x_{t+j} + A_t^*)\right] \cdot \qquad (5.3.19)$$

In general the parameter b_t is given by

$$b_t = \frac{\Delta^L f_{t+2}}{N_t^* \Delta^L \cos(N_t^* x_{t+2} + A_t^*)} \qquad (5.3.20)$$

and the final integration formula is given by

$$y_{t+k} = -\sum_{j=0}^{k-1}\alpha_j\, y_{t+j} + N_t^* h\cdot\sum_{j=0}^{k-1}\beta_j f_{t+j}$$

$$+ \frac{\Delta^L f_{t+2}}{N_t^*\Delta^L \cos(N_t^* x_{t+2}+A_t^*)} \times$$

$$\left[\sum_{j=0}^{k}\alpha_j \sin(N_t^* x_{t+j}+A_t^*) - N_t^* h\sum_{j=0}^{k-1}\beta_j \cos(N_t^* x_{t+j}+A_t^*)\right] \tag{5.3.21}$$

where $\{\beta_j,\ j=0,1,\ldots,k-1\}$ are obtained from the k set of linear equations obtained by setting $i=1,2,\ldots,k$ in equation (5.3.11).

With the consistency parameters $\{\alpha_j, j=0,1,\ldots 4\}$ specified by the equations (5.3.6),(5.3.13) and (5.3.14), the linear multistep scheme given by the equation (5.3.19) is of order 4.

The scheme is also consistent as the consistency parameters have been derived to satisfy the consistency equations (2.4.10) and (2.4.11).

The first characteristic polynomial of the linear multistep scheme given by equation (5.3.19) is

$$\rho(s) = s^4 - s \tag{5.3.22}$$

which has the following roots:

$$s=0,1,\ -\frac{1}{2} \pm i\,\frac{\sqrt{3}}{2}\ . \tag{5.3.23}$$

As all the roots of the first characteristic polynomial of equation (5.3.19) lie within a unit circle and the principal root is a simple root, then by definition (2.4.4), the linear multistep formula (5.3.19) is zero-stable.

From the following theorem of Henrici (1962) which states that the necessary and sufficient condition for a linear multistep scheme to be convergent is that it be consistent and zero-stable, we can rightly assert that the linear multistep scheme given by equation (5.3.19) is convergent.

The parameters N_t^*, A_t^* are used as the initial estimates in the next interval I_{t+1} of integration i.e.

$$N_{t+1}^{[0]} = N_t^* \ , \ t=0,1,\ldots,N-k \tag{5.3.24}$$

$$A_{t+1}^{[0]} = A_t^* \ , \ t=0,1,\ldots,N-k \ . \tag{5.3.25}$$

In the event that the Jacobian of the functions $R_1(N_t,A_t)$ and $R_2(N_t,A_t)$ is singular, a new pair of equations is chosen from equations (5.2.9) to (5.2.11). However, if all possible choices of pairs yield unsatisfactory results, we switch to the alternative interpolating function (5.1.3). A brief discussion on the alternative integration formula based on the interpolating function (5.1.3) will be given in the next section.

5.4 The Alternative Interpolant

In this section, we shall give a brief account of the alternative interpolating function (5.1.3) to the interpolant (5.1.2).

The solution to the initial value problem (5.1.1) is locally represented over the interval I* defined in (5.2.1) by the interpolating function

$$F_t(x) = \sum_{i=0}^{L} a_i x^i + b_t \sinh(N_t x + A_t). \tag{5.4.1}$$

By using the same arguments for the interpolant (5.4.1) as for interpolant (5.1.2), we obtain the following results:

(a) the undetermined coefficient b_t is given by

$$b_t = \frac{\Delta^L f_{t+j}}{N_t \Delta^L \cosh(N_t x_{t+j} + A_t)}, j=0,1,\ldots,k-1, \tag{5.4.2}$$

(b) the parameters N_t and A_t can be obtained from any pair of the following set of functions

$$R_1(N_t,A_t) = \Delta^L \cosh(N_t x_t + A_t).\Delta^L f_{t+1} -$$
$$\Delta^L \cosh(N_t x_{t+1} + A_t).\Delta^L f_t = 0, \tag{5.4.3}$$

$$R_2(N_t,A_t) = \Delta^L \cosh(N_t x_{t+1} + A_t).\Delta^L f_{t+2} -$$
$$\Delta^L \cosh(N_t x_{t+2} + A_t).\Delta^L f_{t+1} = 0, \tag{5.4.4}$$

$$R_3(N_t,A_t) = \Delta^L \cosh(N_t x_{t+2} + A_t).\Delta^L f_t -$$
$$\Delta^L \cosh(N_t x_t + A_t).\Delta^L f_{t+2} = 0. \tag{5.4.5}$$

Equations (5.4.3) to (5.4.5) are obtained by setting j=0,1,2 in equation (5.4.2).

(c) the initial estimates $N_0^{[0]}$ and $A_0^{[0]}$ of the parameters N_0^*, A_0^* are given by either

$$N_0^{[0]} = \left[\frac{\Delta^4 y_0}{\Delta^2 y_0}\right]^{\frac{1}{2}} \qquad (5.4.6)$$

and

$$A_0^{[0]} = \coth^{-1}\left[\frac{\Delta^3 y_0}{N_0^{[0]}.\Delta^2 y_0}\right] - N_0^{[0]}.a \qquad (5.4.7)$$

or by the equations

$$N_0^{[0]} = \left[\frac{\Delta^5 y_0}{\Delta^3 y_0}\right]^{\frac{1}{2}} \qquad (5.4.8)$$

and

$$A_0^{[0]} = \tanh^{-1}\left[\frac{\Delta^4 y_0}{N_0^{[0]}.\Delta^3 y_0}\right] - N_0^{[0]}.a \qquad (5.4.9)$$

Equations (5.4.6) to (5.4.9) are obtained by replacing higher derivatives of $f(x,y)$ in the equations (4.8.2) to (4.8.4) by the equivalent forward differences.

(d) the final integration formula is given by:

$$y_{t+k} = -\sum_{j=0}^{k-1} \alpha_j \; y_{t+j} + h \cdot \sum_{j=0}^{k-1} \beta_j f_{t+j}$$

$$+ \frac{\Delta^L f_{t+2}}{N_t^* \, \Delta^L \cosh(N_t^* x_{t+2} + A_t^*)} \quad x$$

$$\left[\sum_{j=0}^{k} \alpha_j \; \sinh(N_t^* x_{t+j} + A_t^*) - N_t^* h \cdot \sum_{j=0}^{k-1} \beta_j \; \cosh(N_t^* x_{t+j} + A_t^*)\right] \qquad (5.4.10)$$

where

$$N_t^* = \lim_{i\to\infty} N_t^{[i]} \qquad (5.4.11)$$

$$A_t^* = \lim_{i\to\infty} A_t^{[i]} \qquad (5.4.12)$$

and the sequence $\{N_t^{[i]}, A_t^{[i]}, \; i=1,\ldots\}$ are the approximate roots of $R_1(N_t, A_t)$ and $R_2(N_t, A_t)$ which are generated by the

Newton method.

In case the integration formula given by equation (5.4.10) fails because of the parameter N_t vanishing or becoming complex switch to the interpolating function (5.1.2).

5.5 Applications and Numerical Results

Example (5.5.1)

We now consider the scalar initial value problem

$$y' = -\sqrt{1-y^2} \quad , \quad y(a) = \cos a \tag{5.5.1}$$

over the range $\frac{\pi}{10} \leq x \leq \pi$. The theoretical solution of the problem (5.5.1) over the specified range is

$$y(x) = \cos x.$$

The initial estimates of the parameters N_t and A_t are obtained as:

$$N_0^{[0]} = 0.98179374$$
$$A_0^{[0]} = 1.69468235 \quad .$$

The integration was performed with a uniform mesh-size $h = \frac{\pi}{20}$.

The numerical solution was started away from x=0 as the problem (5.5.1) does not satisfy the hypothesis of theorem (1.1) at x=0.

Details of the numerical results are given in table (5.5.1).

TABLE (5.5.1)

$N_0^{[0]} = 0.98179374$

$A_0^{[0]} = 1.69468235$

t	NO. OF NEWTON ITERATIONS	X_t	N^*_t	A^*_t	Y_t	$10^7 x T_{t+1}$
0	4	0.31415926	1.0000007	1.5707955	0.95105652	0.00000
1	2	0.47123889	0.9999989	1.5707974	0.89100654	0.09962
2	2	0.62831852	1.0000032	1.5707919	0.80901702	0.09404
3	2	0.78539815	0.9999985	1.5707986	0.70710681	0.08460
4	1	0.94247778	0.9999985	1.5707986	0.58778529	0.12446
5	2	1.09955741	1.0000037	1.5707909	0.45399054	0.16241
6	2	1.25663704	0.9999943	1.5708053	0.30901705	0.23576
7	1	1.41371667	0.9999940	1.5708057	0.15643451	0.21375
8	2	1.57079630	1.0000026	1.5707921	0.00000005	0.26212
9	2	1.72787593	1.0000002	1.5707961	-0.15643440	0.27809
10	2	1.88495556	0.9999967	1.5708018	-0.30901694	0.17926
11	2	2.04203519	1.0000048	1.5707878	-0.45399044	0.16566
12	2	2.19911482	0.9999967	1.5708028	-0.58778520	0.16873
13	2	2.35619445	0.9999989	1.5707983	-0.70710674	0.09151
14	2	2.51327408	1.0000098	1.5707737	-0.80901695	0.10015
15	-	2.67035371	-	-	-0.89100649	0.07438
16	-	2.82743334	-	-	-0.95105650	0.02741
17	-	2.98451297	-	-	-0.98768832	0.04912
18	-	3.14159265	-	-	-1.00000000	0.07632

Example (5.5.2)

We also consider the initial value problem of Schweitzer(1974) given by:

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \begin{bmatrix} -1 & 1 \\ 1 & -2 \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} + \begin{pmatrix} \sin x \\ 2(\cos x - \sin x) \end{pmatrix},$$

$$\begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{5.5.2}$$

over the range $0 \leq x \leq \pi$.

The theoretical solution to the system (5.5.2) in the specified range is

$$\begin{pmatrix} y_1(x) \\ y_2(x) \end{pmatrix} = \begin{pmatrix} \sin x \\ \cos x \end{pmatrix}.$$

The numerical solution was obtained with a uniform mesh-size $h=\frac{\pi}{20}$.

The initial estimates of the parameters are given as:

$$N_{0,1}^{[0]} = 1.41197420$$

$$A_{0,1}^{[0]} = 0.11112352$$

and

$$N_{0,2}^{[0]} = 0.99505019$$

$$A_{0,2}^{[0]} = 1.68870386.$$

Details of the numerical results are given in tables (5.5.2a) and (5.5.2b).

TABLE (5,5,2a)

t	NO. OF NEWTON ITERATION	X_t	N^*_t	A^*_t	$Y_{t,1}$	$10^7 x T_{t+1,1}$
0	6	0.00000000	1.0000019	0.00000003	0.00000000	0.00000
1	2	0.15707963	1.0000053	-0.00000003	0.15643446	0.04219
2	2	0.31415926	0.9999848	0.00000130	0.30901699	0.09763
3	2	0.47123889	1.0000195	-0.00000393	0.45399050	0.03936
4	2	0.62831852	0.9999779	0.00000785	0.58778524	0.02126
5	2	0.78539815	1.0000256	-0.00001432	0.70710678	0.03520
6	2	0.94247778	0.9999699	0.00002432	0.80901698	0.04340
7	2	1.09955741	1.0000356	-0.00003888	0.89100653	0.05248
8	2	1.25663704	0.9999592	0.00005722	0.95105650	0.06660
9	2	1.41371667	1.0000398	-0.00006932	0.98768835	0.07632
10	2	1.57079630	0.9999651	0.00007132	0.99999998	0.09684
11	2	1.72787593	1.0000469	-0.00010703	0.98768837	0.10978
12	2	1.88495556	0.9999144	0.00021732	0.95105650	0.11948
13	2	2.04203519	1.0001499	-0.00041286	0.819100655	0.033
14	2	2.19911482	0.9997400	0.00075868	0.80901700	0.11045
15	3	2.35619445	1.0004633	-0.00140147	0.70710683	0.14257
16	3	2.51327408	0.9991316	0.00269235	0.58778521	0.48340
17	-	2.67035371	-	-	0.45399064	0.69677
18	-	2.82743334	-	-	0.30901689	1.13746
19	-	2.98451297	-	-	0.15643467	1.13681
20	-	3.14159265	-	-	1.00000000	1.96611

TABLE (5.5.2b)

t	NO.OF NEWTON ITERATION	X_t	$N^*_{t,2}$	$A^*_{t,2}$	$Y_{t,2}$	$10^7 x T_{t+1,2}$
0	4	0.00000000	0.99999996	1.5707963	1.00000000	0.00000
1	2	0.15707963	0.99999962	1.5707984	0.98768834	0.09396
2	2	0.31415926	1.0000151	1.5707818	0.95105651	0.08331
3	2	0.47123889	0.9999735	1.5708279	0.89100652	0.07095
4	2	0.62831852	1.0000408	1.5707412	0.80901700	0.01963
5	2	0.78539815	0.9999343	1.5708924	0.70710678	0.06018
6	2	0.94247778	1.0001147	1.5706209	0.58778527	0.05531
7	2	1.09955741	0.9997664	1.5711613	0.45399050	0.10031
8	2	1.25663704	1.0008089	1.5695258	0.30901703	0.12626
9	2	1.41371667	1.0007450	1.5696261	0.15643447	0.19219
10	3	1.57079630	0.9997980	1.5711155	0.00000005	0.23836
11	2	1.72787593	1.0001824	1.5705043	-0.15643446	0.19378
12	2	1.88495556	0.9997519	1.5712085	-0.30901698	0.11378
13	3	2.04203519	1.0003081	1.5702510	-0.45399052	0.38254
14	3	2.19911482	0.9996277	1.5715125	-0.58778516	0.38153
15	3	2.35619445	1.0004596	1.5698189	-0.70710686	0.62036
16	3	2.51327408	0.9994182	1.5721769	-0.80901686	0.62575
17	-	2.67035371	-	-	-0.89100667	0.88692
18	-	2.82743334	-	-	-0.95105628	1.11933
19	-	2.98451297	-	-	-0.98768865	1.61092
20	-	3.14159265	-	-	-1.00000000	2.10282

Example (5.5.3)

We also consider the system

$$\begin{pmatrix} y_1' \\ \\ y_2' \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \\ -\frac{\beta^2}{x^2} & -\frac{1}{x} \end{pmatrix} \begin{pmatrix} y_1 \\ \\ y_2 \end{pmatrix} \qquad (5.5.3)$$

over the interval $7.38905610 \leq x \leq 8.98905610$ with initial conditions

$$y_1(a) = 1$$

$$y_2(a) = 0.42516833$$

where $a = 7.38905610$.

The computation was completed with a uniform mesh size of $h=0.1$. The initial estimates of parameters are given by

$$N_{0,1}^{[0]} = 0.45730571$$

$$A_{0,1}^{[0]} = -1.68002638$$

and

$$N_{0,2}^{[0]} = 1.96633719$$

$$A_{0,2}^{[0]} = -14.04732875 .$$

Details of the numerical results are given in tables (5.5.3.a) and (5.5.3b).

TABLE (5.5.3a)

$N_{0,1}^{[0]} = 0.45730571$

$A_{0,1}^{[0]} = -1.68002638$

NO.OF NEWTON ITERATIONS	t	X_t	$N^*_{t,1}$	A^*_t	$Y_{t,1}$	$10^6 x T_{t+1}$
4	0	7.38905610	0.4356458	-1.5280714	1.00000000	0.00000
6	1	7.48905610	0.4119962	-1.3370577	1.04132752	0.00418
9	2	7.58905610	0.3998252	-1.2359248	1.08028699	0.00527
9	3	7.68905610	0.3700663	-0.9810982	1.11689773	0.00623
13	4	7.78905610	0.3517235	-0.8190168	1.15118345	0.06750
16	5	7.88905610	0.3426462	-0.7366731	1.18317107	0.00196
8	6	7.98905610	0.3113717	-0.4442881	1.21289184	0.03444
15	7	8.08905610	0.2944521	-0.2809082	1.24037929	0.05815
3	8	8.18905610	0.2883406	-0.2205216	1.26566957	0.04245
9	9	8.28905610	0.2531217	0.1379613	1.28880209	0.03104
4	10	8.38905610	0.2371443	0.3060069	1.30981705	0.01801
11	11	8.48905610	0.2341942	0.3376040	1.32875693	0.11055
8	12	8.58905610	0.1905928	0.8182852	1.34566660	0.00710
-	13	8.68905610	-	-	1.36059045	0.03971
-	14	8.78905610	-	-	1.37357500	0.19191
-	15	8.88905610	-	-	1.38466850	0.02773
-	16	8.98905510	-	-	1.39391758	0.10814

TABLE (5.5.3b)

$$N^{[0]}_{0,2} = 1.96633719$$

$$A^{[0]}_{0,2} = -14.04732875$$

NO. OF NEWTON ITERATIONS	t	X_t	$N^*_{t,2}$	$A^*_{t,2}$	$Y_{t,2}$	$10^6 x T_{t+1}$
6	0	7.38905610	1.5760359	-11.2858253	0.42516833	0.00000
5	1	7.48905610	1.3724154	-9.8070483	0.40140655	0.00329
5	2	7.58905610	1.2262821	-8.7393236	0.37781517	0.00329
5	3	7.68905610	1.1109863	-7.8907389	0.35443898	0.00329
5	4	7.78905610	1.0175952	-7.1975520	0.33131763	0.36287
4	5	7.88905610	0.9436730	-6.6435050	0.30848809	0.26902
4	6	7.98905610	0.8771 44	-6.1393280	0.28598162	0.21651
4	7	8.08905610	0.8182216	-5.6876621	0.26382606	0.55344
4	8	8.18905610	0.7721938	-5.3301387	0.24204741	0.41530
4	9	8.28905610	0.7261200	-4.9671397	0.22066680	0.34360
4	10	8.38905610	0.6827084	-4.6200680	0.19970275	0.68269
10	11	8.48905610	0.6514154	-4.365 428	0.17917270	0.50778
4	12	8.58905610	0.6159374	-4.0726420	0.15908980	0.42887
-	13	8.68905610	-	-	0.13946534	0.77925
-	14	8.78905610	-	-	0.12031009	0.56714
-	15	8.88905610	-	-	0.10163100	0.48782
-	16	8.98905610	-	-	0.08343378	0.85443

We also obtained the numerical solution to the initial value problem (5.5.3) using the following numerical integration schemes:

(a) the variable order Gragg-Bulirsch-Stoer algorithm with orders in the range $6 \leq M \leq 8$.

(b) Krogh's variable order Adams method and

(c) the one-step scheme proposed in chapter IV.

Apart from Krogh's algorithm which requires a very small mesh-size to generate the required starting values, the integration procedures were carried out with a uniform mesh size of h=0.05.

The details of the numerical results are given in Tables (5.5.3c) to (5.5.3f).

Whilst the one-step scheme proposed in chapter IV compares favourably with Krogh's scheme in terms of efficiency and accuracy, the linear multistep scheme proposed in this chapter has a smaller truncation error than the variable order Gragg-Bulirsch-Stoer algorithm despite the fact that the degree of accuracy in this scheme is limited by the accuracy to which the oscillatory parameters N_t^* and A_t^* are obtained.

<u>TABLE (5.5.3c)</u>

GRAGG-BULIRSCH-STOER RATIONAL EXTRAPOLATION SCHEME

ORDER M: 6≤M≤8

H=0.05

X	Y_1	Y_2	$10^8 x T_1$	$10^8 x T_2$
7.38905610	1.00000000	0.42516833	0.00000	0.00000
7.48905610	1.04132749	0.40140654	0.21539	0.61680
7.58905610	1.08028699	0.37781517	0.32178	0.95133
7.68905610	1.11689773	0.35443898	0.18698	1.28228
7.78905610	1.15118329	0.33131809	0.43699	1.61252
7.88905610	1.18317105	0.30848842	0.72587	1.92924
7.98905610	1.21289174	0.28598187	1.03045	2.24703
8.08905610	1.24037913	0.26382672	1.36791	2.5449
8.18905610	1.26566962	0.24204789	1.72773	2.83207
8.28905610	1.28880197	0.22066718	2.10128	3.11458
8.38905610	1.30981695	0.19970353	2.49607	3.37703
8.48905610	1.32875712	0.17917326	2.89631	3.63112
8.58905610	1.34566651	0.15909026	3.31714	3.86164
8.68905610	1.36059045	0.13946618	3.74680	4.08938
8.78905610	1.37357535	0.12031068	4.18672	4.28416
8.88905610	1.38466846	0.10163149	4.63651	4.47329
8.98905610	1.39391772	0.08343466	5.08666	4.64193

TABLE (5.5.3d)

KROGH's VARIABLE ORDER ADAM's

H	X	Y_1	Y_2	$10^8 x T_1$	$10^8 x T_2$
0.00625	7.38905610	1.00000000	0.42516833	0.00000	0.00000
0.01250	7.48905610	1.04132752	0.40140655	0.32222	0.28893
0.02500	7.58905610	1.08028700	0.37781517	0.29030	0.29546
0.05000	7.68905610	1.11689774	0.35443898	0.26328	0.30217
0.05000	7.78905610	1.15118331	0.33131811	0.24353	0.31370
0.05000	7.88905610	1.18317107	0.30848844	0.21596	0.31750
0.05000	7.98905610	1.21289177	0.28598189	0.19991	0.33042
0.05000	8.08905610	1.24037916	0.26383675	0.17667	0.33276
0.05000	8.18905610	1.26566967	0.24204792	0.15350	0.33537
0.05000	8.28905610	1.28880202	0.22066722	0.13606	0.34482
0.05000	8.38905610	1.30981701	0.19970357	0.11214	0.34691
0.05000	8.48905610	1.32875719	0.17917330	0.09748	0.35387
0.05000	8.58905610	1.34566659	0.15909030	0.07569	0.35153
0.05000	8.68905610	1.36059054	0.13946623	0.05795	0.36125
0.0500	8.78905610	1.37357545	0.12031072	0.03985	0.35339
0.05000	8.88905610	1.38466857	0.10163153	0.02014	0.35641
0.05000	8.98905610	1.39391784	0.08343471	0.00426	0.35971

TABLE (5.5.3e)

FOURTH ORDER ONE STEP FORMULA (CHAPTER IV)

H=0.05

X	Y_1	Y_2	$10^8 xT_1$	$10^8 xT_2$
7.38905610	1.00000000	0.42516833	0.00000	0.00000
7.48905610	1.0413275	0.40140655	0.33077	0.37823
7.58905610	1.0802870	0.37781519	0.30289	0.44596
7.68905610	1.1168977	0.35443898	0.27497	0.49852
7.78905610	1.1511833	0.33131810	0.25029	0.54598
7.88905610	1.1831711	0.30848843	0.21396	0.57941
7.98905610	1.2128918	0.28598189	0.18873	0.61756
8.08905610	1.2403792	0.26382675	0.15524	0.64134
8.18905610	1.2656697	0.24204792	0.12203	0.66269
8.28905610	1.2888020	0.22066721	0.09028	0.68845
8.38905610	1.3098170	0.19970357	0.05103	0.70443
8.48905610	1.3287572	0.17917329	0.01875	0.73263
8.58905610	1.3456666	0.15909029	0.01799	0.73162
8.68905610	1.3605905	0.13946622	0.05117	0.75029
8.78905610	1.3735754	0.12031072	0.08706	0.75037
8.88905610	1.3939178	0.08343470	0.15622	0.76407

TABLE (5.5.3f)

LINEAR MULTISTEP SCHEME (CHAPTER V)

H=0.05

X	Y_1	Y_2	$10^8 xT_1$	$10^8 xT_2$
7.38905610	1.00000000	0.42516833	0.00000	0.00000
7.48905610	1.04132751	0.40140654	0.85544	0.65911
7.58905610	1.08028700	0.37781515	0.30569	0.188604
7.68905610	1.11689772	0.35443896	0.25641	1.79557
7.78905610	1.15118330	0.33131808	0.08997	2.62959
7.88905610	1.18317107	0.30848840	0.21996	3.46230
7.98905610	1.21289176	0.28598186	0.34853	3.02981
8.08905610	1.24037915	0.26382671	0.42479	3.68022
8.18905610	1.26566966	0.24204787	0.11111	4.38708
8.28905610	1.28880200	0.22066717	0.65359	3.76385
8.38905610	1.30981699	0.19970352	0.92547	4.34148
8.48905610	1.32875717	0.17917324	0.57051	5.01575
8.58905610	1.34566656	0.15909025	1.06394	4.23388
8.68905610	1.36059051	0.13946618	1.50476	4.77740
8.78905610	1.37357542	0.12031066	1.11397	5.44368
8.88905610	1.38466853	0.10163149	1.54571	4.53306
8.98905610	1.39391778	0.08343466	2.28377	5.01751

Chapter VI

A LINEAR MULTISTEP SCHEME FOR SOLVING A SPECIAL CLASS OF SECOND ORDER DIFFERENTIAL EQUATIONS WITH OSCILLATORY SOLUTIONS

6.1 INTRODUCTION

Shaw (1967) proposed a multistep integration formula for solving initial value problems of the form

$$y^{(r)} = f(x,y) \,, \qquad (6.1.1)$$
$$y^{(i)}(a) = \eta_i, \ i=0,1,\ldots,r-1 \text{ for } r\geq 1.$$

The numerical integration procedure was based on the representation of the solution y(x) to problem (6.1.1) by the interpolating function

$$F(x) = \sum_{i=0}^{L+1} a_i x^i \ , \ L+1\geq r \qquad (6.1.2)$$

and is particularly well suited to systems of ordinary differential equations whose solutions contain singularities.

Henrici (1962) and Lambert (1973) both discussed linear multistep methods for obtaining the numerical solutions of second order ordinary differential equations in the form (6.1.1). The linear k-step methods are of the form:

$$\sum_{j=0}^{k} \alpha_j y_{t+j} = h^2 \sum_{j=0}^{k} \beta_j f_{t+j} \qquad (6.1.3)$$

where $\alpha_k = +1$ and $|\alpha_0|+|\beta_0|>0$.

In chapter V, we proposed a linear multistep scheme for integrating systems of the form,

$$y' = f(x,y), \ y(a) = \eta \ , \qquad (6.1.4)$$

whose solutions are known to be oscillatory. The integration scheme was based on the local representation of the solution to (6.1.4) by either a combination of a polynomial and trigonometric function or a polynomial and hyperbolic function. This approach requires a transformation of the second order differential equation

$$y'' = f(x,y) \tag{6.1.5}$$

into a first order system $u'=v$; $v'=f(x,u,v)$ where $u=y$ and $v=y'$. The introduction of the first derivative explicitly into an equation in which it does not appear approximately doubles the amount of computation. The increase in the computation can increase the tendency of the propagation of round off errors. For the sake of computational efficiency and to achieve a higher degree of accuracy, we shall use a similar approach as in chapter V to develop a linear multistep scheme to integrate directly special second order systems of the form (6.1.5) whose solutions are known to be of an oscillatory nature.

6.2 THE INTERPOLATING FUNCTION AND THE DETERMINATION OF THE PARAMETERS N_T AND A_T

We shall denote by k, the step-number of the linear multistep scheme to solve the initial value problem

$$y'' = f(x,y) \; , \qquad y(a) = \eta \; , \qquad y'(a) = \eta^* \; . \tag{6.2.1}$$

The necessary additional starting values $\{y_1, y_2, \ldots\ldots, y_{k-1}\}$ are obtained by the variable order Gragg-Bulirsch-Stoer algorithm as discussed in chapter III.

In order to obtain the numerical solution y_{t+k} at $x=x_{t+k}$, the solution to problem (6.2.1) is locally represented over the interval

$$I^* = \bigcup_{i=0}^{k-1} I_{t+i} \tag{6.2.2}$$

by the interpolating function

$$F_t(x) = \sum_{r=0}^{L+1} a_r x^r + b_t \sin(N_t x + A_t), L \geq 1 \tag{6.2.3}$$

where L is a positive integer, b_t and $\{a_r, r=0,1,\ldots,L+1\}$ are real undetermined coefficients whilst N_t and A_t are the oscillatory parameters whose values are obtained to a specified degree of accuracy at each step of the integration procedure.

As the interpolating function (6.2.3) is required to pass through the points $\{(x_{t+j}, y_{t+j}), j=0,1,\ldots,k\}$, the first set of constraints on the interpolant are then given by

$$F_t(x)\Big|_{x=x_{t+j}} = \sum_{r=0}^{L+1} a_r x_{t+j}^r + b_t \sin(N_t x_{t+j} + A_t) = y_{t+j} \, , \quad j=0,1,\ldots,k. \tag{6.2.4}$$

The interpolating function (6.2.6) is also expected to satisfy the differential equation (6.2.1) at the mesh points $\{x_{t+j},\ j=0,1,\dots,k\}$. Hence the second set of constraints are given by

$$\left.\frac{d^2F_t(x)}{dx^2}\right|_{x=x_{t+j}} = \sum_{i=0}^{L+1} i(i-1)a_i x_{t+j}^{i-2} - N_t^2 b_t \sin(N_t x_{t+j}+A_t)=f_{t+j},$$

$$j=0,1,\dots,k-1 \quad . \qquad (6.2.5)$$

According to theorem (2.1), the L^{th} forward difference will annihilate all polynomials of degree less than L. Hence, applying the operator Δ^L to both sides of equation (6.2.5) gives the relationship:

$$\Delta^L f_{t+j} = -N_t^2 b_t \Delta^L \sin(N_t x_{t+j}+A_t),\ j=0,1,\dots,k-1. \qquad (6.2.6)$$

Equation (6.2.6) implies that,

$$b_t = \frac{-\Delta^L f_{t+j}}{N_t^2 \Delta^L \sin(N_t x_{t+j}+A_t)},\ j=0,1,\dots,k-1. \ (6.2.7)$$

In particular, for j=0,1,2 we have

$$b_t = \frac{-\Delta^L f_t}{N_t^2\ \Delta^L \sin(N_t x_t+A_t)}$$

$$= \frac{-\Delta^L f_{t+1}}{N_t^2\ \Delta^L \sin(N_t x_{t+1}+A_t)}$$

$$= \frac{-\Delta^L f_{t+2}}{N_t^2\ \Delta^L \sin(N_t x_{t+2}+A_t)} \quad . \qquad (6.2.8)$$

From equation (6.2.8) we obtain the following three trigonometric functions in the parameters N_t and A_t:

$$R_1(N_t,A_t) = \Delta^L f_t . \Delta^L \sin(N_t x_{t+1}+A_t) - \Delta^L f_{t+1} . \Delta^L \sin(N_t x_t + A_t) = 0, \tag{6.2.9}$$

$$R_2(N_t,A_t) = \Delta^L f_{t+1} . \Delta^L \sin(N_t x_{t+2}+A_t) - \Delta^L f_{t+2} . \Delta^L \sin(N_t x_{t+1} + A_t) = 0, \tag{6.2.10}$$

and finally,

$$R_3(N_t,A_t) = \Delta^L f_{t+2} . \Delta^L \sin(N_t x_t+A_t) - \Delta^L f_t . \Delta^L \sin(N_t x_{t+2} + A_t) = 0 \ . \tag{6.2.11}$$

The values of the parameters N_t^* and A_t^* can be obtained by using any of the standard algorithms for solving systems of nonlinear equations in any pair of the equations (6.2.9) to (6.2.11). For example, we shall adopt the Newton iteration scheme to obtain the roots N_t^* and A_t^* from equations (6.2.9) and (6.2.10) for the case L=1 and k=4.

Equation (6.2.9) is now given by:

$$\begin{aligned} R_1(N_t,A_t) = {} & (f_{t+2}-f_{t+1})\left[\sin(N_t x_t+A_t)-\sin(N_t x_{t+1}+A_t)\right] - \\ & (f_{t+1}-f_t)\left[\sin(N_t x_{t+1}+A_t)-\sin(N_t x_{t+2}+A_t)\right]=0 \end{aligned} \tag{6.2.12}$$

and

$$\begin{aligned} R_2(N_t,A_t) = {} & (f_{t+3}-f_{t+2})\left[\sin(N_t x_{t+1}+A_t)-\sin(N_t x_{t+2}+A_t)\right] \\ & -(f_{t+2}-f_{t+1})\left[\sin(N_t x_{t+2}+A_t)-\sin(N_t x_{t+3}+A_t)\right]=0 . \end{aligned} \tag{6.2.13}$$

We denote the partial derivatives of $R_1(N_t,A_t)$ and $R_2(N_t,A_t)$ with respect to the parameters N_t and A_t as follows:

$$R_{1,N_t} = \frac{\partial R_1(N_t,A_t)}{\partial N_t} \ , \ R_{2,N_t} = \frac{\partial R_2(N_t,A_t)}{\partial N_t} \ ,$$

$$R_{1,A_t} = \frac{\partial R_1(N_t,A_t)}{\partial A_t} \ \text{and} \ R_{2,A_t} = \frac{\partial R_2(N_t,A_t)}{\partial A_t} \ .$$

From equation (6.2.12) and (6.2.13), these partial derivatives are given as follows:

$$R_{1,N_t} = (f_{t+2}-f_{t+1})\left[x_t\cos(N_t x_t+A_t)-x_{t+1}\cos(N_t x_{t+1}+A_t)\right]$$
$$-(f_{t+1}-f_t)\left[x_{t+1}\cos(N_t x_{t+1}+A_t)-x_{t+2}\cos(N_t x_{t+2}+A_t)\right], \quad (6.2.14)$$

$$R_{2,N_t} = (f_{t+3}-f_{t+2})\left[x_{t+1}\cos(N_t x_{t+1}+A_t)-x_{t+2}\cos(N_t x_{t+2}+A_t)\right]$$
$$-(f_{t+2}-f_{t+1})\left[x_{t+2}\cos(N_t x_{t+2}+A_t)-x_{t+3}\cos(N_t x_{t+3}+A_t)\right], \quad (6.2.15)$$

$$R_{1,A_t} = (f_{t+2}-f_{t+1})\left[\cos(N_t x_t+A_t)-\cos(N_t x_{t+1}+A_t)\right]$$
$$-(f_{t+1}-f_t)\left[\cos(N_t x_{t+1}+A_t)-\cos(N_t x_{t+2}+A_t)\right], \quad (6.2.16)$$

and finally,

$$R_{2,A_t} = (f_{t+3}-f_{t+2})\left[\cos(N_t x_{t+1}+A_t)-\cos(N_t x_{t+2}+A_t)\right]$$
$$-(f_{t+2}-f_{t+1})\left[\cos(N_t x_{t+2}+A_t)-\cos(N_t x_{t+3}+A_t)\right]. \quad (6.2.17)$$

Let $N_t^{[i]}$ and $A_t^{[i]}$ denote the estimates of the roots N_t^* and A_t^* at the i^{th} iteration of the Newton Raphson root finding scheme, and $R_{1,N_t}^{[i]}$, $R_{2,N_t}^{[i]}$, $R_{1,A_t}^{[i]}$ and $R_{2,A_t}^{[i]}$ denote the partial derivatives of the functions $R_1(N_t,A_t)$ and $R_2(N_t,A_t)$ at $N_t=N_t^{[i]}$ and $A_t=A_t^{[i]}$. The determinant of the Jacobian J of the functions $R_1(N_t,A_t)$ and $R_2(N_t,A_t)$ is denoted by J and given by

$$J = \begin{vmatrix} R_{1,N_t}^{[i]} & R_{1,A_t}^{[i]} \\ R_{2,N_t}^{[i]} & R_{2,A_t}^{[i]} \end{vmatrix} . \quad (6.2.18)$$

The correction terms $\delta N_t^{[i]}$, $\delta A_t^{[i]}$ are obtained as

$$\begin{bmatrix} \delta N_t^{[i]} \\ \delta A_t^{[i]} \end{bmatrix} = -J^{-1} \begin{bmatrix} R_{2,A_t}^{[i]} & -R_{2,N_t}^{[i]} \\ -R_{1,A_t}^{[i]} & R_{1,N_t}^{[i]} \end{bmatrix} \begin{bmatrix} R_1^{[i]} \\ R_2^{[i]} \end{bmatrix} \quad (6.2.19)$$

where

$$R_1^{[i]} = R_1(N_t^{[i]}, A_t^{[i]}) \ , \quad (6.2.20)$$

and

$$R_2^{[i]} = R_2(N_t^{[i]}, A_t^{[i]}) \ . \quad (6.2.21)$$

The improved parameters are expressed as:

$$N_t^{[i+1]} = N_t^{[i]} + \delta N_t^{[i]} , \quad (6.2.22)$$

and

$$A_t^{[i+1]} = A_t^{[i]} + \delta A_t^{[i]} . \quad (6.2.23)$$

If we define the corrector vector $\delta \underline{\alpha}$ as:

$$\delta \underline{\alpha} = (\delta N_t^{[i]}, \delta A_t^{[i]})^T \quad (6.2.24)$$

the Newton iteration is halted when

$$||\delta \underline{\alpha}|| < \varepsilon_{max} ,$$

where ε_{max} is the allowable tolerance.

The limiting values of the parameters are then given as:

$$N_t^* = \lim_{i \to \infty} N_t^{[i]} , \quad (6.2.25)$$

and

$$A_t^* = \lim_{i \to \infty} A_t^{[i]} . \quad (6.2.26)$$

As it is desirable to have good initial estimates $N_0^{[0]}$, $A_0^{[0]}$ of the parameters N_t^* and A_t^* in order to ascertain the convergence of the Newton's iteration, we propose a scheme similar to the one used in chapter V.

The initial estimates $N_0^{[0]}$ and $A_0^{[0]}$ are obtained from equations (4.4.13) to (4.4.15) and are given by either

$$N_0^{[0]} = \left[-\frac{\Delta^4 y_0}{\Delta^2 y_0} \right]^{\frac{1}{2}} , \tag{6.2.27}$$

and

$$A_0^{[0]} = \cot^{-1} \left[\frac{\Delta^3 y_0}{N_0^{[0]} . \Delta^2 y_0} \right] - N_0^{[0]} . a \tag{6.2.28}$$

or

$$N_0^{[0]} = \left[-\frac{\Delta^5 y_0}{\Delta^3 y_0} \right]^{\frac{1}{2}} , \tag{6.2.29}$$

and

$$A_0^{[0]} = \tan^{-1} \left[\frac{\Delta^4 y_0}{N_0^{[0]} . \Delta^3 y_0} \right] - N_0^{[0]} . a \quad . \tag{6.2.30}$$

The starting values of the multistep scheme which are generated by the variable order Gragg-Bulirsch-Stoer algorithm are used in equations (6.2.27) to (6.2.30).

The approximate roots N_t^* and A_t^* given by equation (6.2.25) and (6.2.26) will be used in the final integration formula to obtain the numerical solution y_{t+k} at $x=x_{t+k}$, $t \geq 0$. The derivation of the integration formula will be discussed in the next section.

6.3 THE DERIVATION OF THE INTEGRATION FORMULAE

In this section, we shall eliminate the undetermined coefficients $\{a_r, r=0,1,\ldots,L+1\}$ in the interpolating function (6.2.4) as well as to obtain values for the consistency parameters $\{\alpha_j,\beta_j;\ j=0,1,\ldots,k\}$. These parameters are determined so as to ensure the consistency and zero-stability of the resultant linear multistep formula for solving the initial value problems of the form (6.2.1) whose solutions are oscillatory.

Let the function z_{t+i} be defined as:

$$z_{t+i} = y_{t+i} - b_t \sin(N_t x_{t+i} + A_t) . \qquad (6.3.1)$$

The second derivative z''_{t+i} of z_{t+i} is then given by

$$z''_{t+i} = f_{t+i} + N_t^2 b_t \sin(N_t x_{t+i} + A_t) . \qquad (6.3.2)$$

We now combine equations (6.3.1) and (6.3.2) with equations (6.2.4) and (6.2.5) to obtain

$$z_{t+i} = \sum_{i=0}^{L+1} a_i x_{t+j}^{i} , \qquad (6.3.3)$$

and

$$z''_{t+i} = \sum_{i=0}^{L+1} i(i-1) a_i x_{t+j}^{i-2} . \qquad (6.3.4)$$

We shall now use equations (6.3.3) and (6.3.4) to generate the consistency parameters $\{\alpha_j,\beta_j;j=0,1,\ldots,k\}$. At the moment, we only know that these parameters are real numbers. For $j=0,1,\ldots,k$; we multiply equation (6.3.3) by α_j and equation (6.3.4) by $-h^2\beta_j$ and add columnwise to obtain

$$\sum_{j=0}^{k} \alpha_j z_{t+j} - h^2 \sum_{j=0}^{k} \beta_j z''_{t+j}$$

$$= \sum_{i=0}^{L+1} a_i \left[\sum_{j=0}^{k} \alpha_j x_{t+j}^{i} - h^2 \sum_{j=0}^{k} i(i-1)\beta_j x_{t+j}^{i-2} \right] . \qquad (6.3.5)$$

Since we are only interested in an explicit scheme, β_k is set to zero. It is also assumed that $\alpha_k \neq 0$ and that $|\alpha_0|+|\beta_0|>0$.

With consistency criteria in mind, the parameters $\{\alpha_j, j=0,1.,,..,k\}$ are obtained from the following equations:

$$\sum_{j=0}^{k} \alpha_j = 0 \ , \tag{6.3.6}$$

and

$$\sum_{j=0}^{k} j\alpha_j = 0 \ . \tag{6.3.7}$$

For the case L=1 and k=4, equations (6.3.6) and (6.3.7) constitute a linear system containing two equations and five unknowns $\alpha_0, \alpha_1, \alpha_2, \alpha_3$ and α_4. As the system is under-determined, we have three degrees of freedom. In all practical applications, we set

$$\alpha_0 = 0 \ ,$$

$$\alpha_2 = 0 \ ,$$

and

$$\alpha_4 = +1. \tag{6.3.8}$$

By using the values in equation (6.3.8) in equations (6.3.6) and (6.3.7), we obtain

$$\alpha_1 = 0.5 \ ,$$

$$\alpha_3 = -1.5 \ . \tag{6.3.9}$$

By using equations (6.3.6) and (6.3.7) in equation (6.3.5), the coefficients of a_0 and a_1 vanish and equation (6.3.5) is reduced to the form

$$\sum_{j=0}^{k} \alpha_j z_{t+j} - h^2 \sum_{j=0}^{k-1} \beta_j z''_{t+j}$$

$$= \sum_{i=2}^{L+1} a_i \left[\sum_{j=0}^{k} \alpha_j x^i_{t+j} - h^2 \sum_{j=0}^{k-1} i(i-1)\beta_j x^{i-2}_{t+j}\right] . \tag{6.3.10}$$

We still have to determine the parameters $\beta_0, \beta_1, \beta_2$, and β_3. There is no loss of generality in setting the coefficients of a_2, a_3, a_4 and a_5 to zero in equation (6.3.10). This gives

$$\sum_{j=0}^{k} \alpha_j x_{t+j}^{i} = h^2 \sum_{j=0}^{k-1} i(i-1)\beta_j x_{t+j}^{i-2} \;, \; i=2,3,4,5 \;. \qquad (6.3.11)$$

We now set $h=1$ and $x_t=0$ in equation (6.3.11) to obtain

$$\sum_{j=0}^{k} j^i \alpha_j = \sum_{j=0}^{k-1} i(i-1)\beta_j \, j^{i-2}, \; i=2,3,4,5 \quad . \qquad (6.3.12)$$

The system of linear equations (6.3.12) is solved to give:

$$\beta_0 = -0.083333$$

$$\beta_1 = 0.375$$

$$\beta_2 = 0 \qquad (6.3.13)$$

and $$\beta_3 = 1.208333 \quad .$$

This procedure makes equation (6.3.10) an explicit linear multistep formula with an associated linear equation $\mathcal{L}$ which can be written as

$$\mathcal{L}[z(x);h] = \sum_{j=0}^{k}\alpha_j z(x+jh) - h^2 \cdot \sum_{j=0}^{k-1} \beta_j z''(x+jh), \qquad (6.3.14)$$

for an arbitrary function $z(x) \in C^{\infty}[a,b]$.

On obtaining the Taylor's expansion of $z(x+jh)$ and $z''(x+jh)$ about the point x and substituting in equation (6.3.14) to give,

$$\mathcal{L}[z(x);h] = c_0 z(x) + c_1 h z^{(1)}(x) + \ldots + c_r h^r z^{(r)}(x) + \ldots \qquad (6.3.15)$$

where

$$c_0 = \sum_{j=0}^{k} \alpha_j,$$

$$c_1 = \sum_{j=0}^{k} j\alpha_j \;, \qquad (6.3.16)$$

$$c_2 = \frac{1}{2!}\sum_{i=1}^{k} j^2\ \alpha_j - \sum_{j=0}^{k}\beta_j ,$$

$$c_r = \frac{1}{r!}\sum_{j=0}^{k} j^r\alpha_j - \frac{1}{(r-2)!}\sum_{j=1}^{k-1} j^{r-2}\beta_j \ ,r=2,3,\ldots \quad .$$

The constants c_r, $r=0,1,\ldots$ will be used later in determining the order and convergence properties of the linear multistep formula.

From equation (6.2.7), we can obtain the parameter b_t as

$$b_t = \frac{-(f_{t+3}-f_{t+2})}{N_t^2\left[\sin(N_t x_{t+3}+A_t)-\sin(N_t x_{t+2}+A_t)\right]} \ . \quad (6.3.17)$$

We can now write equation (6.3.10) with the coefficients of $\{a_i,\ i=0,1,\ldots,L+1\}$ set to zero i.e., the right hand side of equation (6.3.10) vanishes identically. Hence we have:

$$\sum_{j=0}^{k}\alpha_j z_{t+j} - h^2 \sum_{j=0}^{k-1}\beta_j z''_{t+j} \quad = 0 . \quad (6.3.18)$$

By using equations (6.3.1) and (6.3.2) in equation (6.3.18), we obtain

$$\sum_{j=0}^{k}\alpha_j\left[y_{t+j}-b_t\sin(N_t^*x_{t+j}+A_t^*)\right]$$

$$-h^2\sum_{j=0}^{k-1}\beta_j\left[f_{t+j}+N_t^{*2}b_t\sin(N_t^*x_{t+j}+A_t^*)\right] = 0 \quad . \quad (6.3.19)$$

We eliminate the parameter b_t from equation (6.3.19) by using equation (6.3.17). The final integration formula is now given by

$$y_{t+k} = -\sum_{j=0}^{k-1}\alpha_j y_{t+j} - h^2\sum_{j=0}^{k-1}\beta_j f_{t+j}$$

$$+\frac{(f_{t+3}-f_{t+2})}{N_t^{*2}\left[\sin(N_t^* x_{t+3}+A_t^*)-\sin(N_t^* x_{t+2}+A_t^*)\right]} \; x$$

$$\left[\sum_{j=0}^{k}\alpha_j \sin(N_t^* x_{t+j}+A_t^*) + N_t^{*2}\, h^2 \sum_{j=0}^{k-1}\beta_j \sin(N_t^* x_{t+j}+A_t^*)\right] . \tag{6.3.20}$$

According to Henrici (1962), the explicit linear multistep formula (6.3.20) together with the linear operator $\mathcal{L}$ is said to be of order p if the constants c_r, r=0,1,... defined by equations (6.3.16) are such that

$$c_r = 0 \text{ for } r \leq p+1$$

and $c_{p+2} \neq 0$. (6.3.21)

Hence the linear multistep scheme (6.3.20) obtained by setting L=1 and k=4 is of order p=4.

The linear multistep method given by equation (6.3.20) is said to be convergent if for all functions f=f(x,y) satisfying the conditions of theorem (1.1) and all constants η, η^*;

if y(x) is the solution to the initial value problem (6.2.1) such $y(a) = \eta$; $y'(a) = \eta^*$,

$$\lim_{\substack{h\to 0\\ x_t \to x}} y_t = y(x) \tag{6.3.22}$$

holds for all $x \in [a,b]$ and for all sequences $\{y_t\}$ defined by equation (6.3.20) with the starting values $y_\mu = \eta_\mu(h)$ satisfying the conditions

$$\lim_{h\to 0} \eta_\mu(h) = \eta,$$

and

$$\lim_{h\to 0} \frac{\eta_\mu(h)-\eta_0(h)}{\mu h} = \eta^*. \tag{6.3.23}$$

for $\mu = 0,1,\ldots,k-1$.

We now define the first and second characteristic polynomials of the linear multistep method as follows:

$$\rho(s) = \sum_{j=0}^{k} \alpha_j s^j \tag{6.3.24}$$

and

$$\sigma(s) = \sum_{j=0}^{k} \beta_j s^j \quad . \tag{6.3.25}$$

The method is said to be consistent if it is at least of order p=1 i.e. $c_o = c_1 = c_2 = 0$. This implies that,

$$\rho(1) = \rho'(1) = 0,$$

and $$\rho''(1) = 2\sigma(1) \quad . \tag{6.3.26}$$

The first consistency condition in equation (6.2.26) indicates that the first characteristic polynomial of a consistent linear multistep method should have a repeated root at s=+1.

If we now use equations (6.3.8) and (6.3.9) in equation (6.3.24), we have

$$\rho(s) = \frac{1}{2}(2s^4 - 3s^3 + s) \quad , \tag{6.3.27}$$

whose roots are

$$s = +1(\text{double}),\ s=0 \text{ and } s= -\frac{1}{2} \quad . \tag{6.3.28}$$

Also, we have that $\rho''(1) = 2\sigma(1)$. Hence, the linear multistep formula (6.3.20) is consistent.

The linear multistep method (6.3.20) is said to be zero-stable if no root of the first characteristic polynomial $\rho(s)$ has modulus greater than one, and if every root of modulus unity has multiplicity not exceeding two.

From equations (6.3.27) and (6.3.28) we observe that linear multistep formula (6.3.20) is zero stable and hence by a theorem in Henrici (1962), the formula (6.3.20) is convergent.

In the event that the interpolating function (6.2.3) proves unsatisfactory as a result of the parameter N_t^* vanishing or becoming infinite or complex, a new pair of equations is chosen from equations (6.2.9) to (6.2.11). However if all possible pairs of equations fail to give the desirable values of N_t^* and A_t^*, the alternative interpolant to be considered in the next section can be applied.

6.4 THE ALTERNATIVE INTERPOLATING FUNCTION

In the event that the interpolating function (6.2.3) is unsuitable, we introduce the alternative interpolant:

$$F_t(x) = \sum_{r=0}^{L+1} a_r x^r + b_t \sinh(N_t x + A_t) \quad . \tag{6.4.1}$$

The undetermined coefficients $b_t, \{a_r, r=0,1,\ldots,L+1\}$ as well as the parameters N_t and A_t are identical to those of the interpolating function (6.2.3).

By adopting an identical procedure as in sections (6.2) and (6.3) to the interpolating function (6.4.1), we obtain the following results:

(a) The parameter b_t is now given by:

$$b_t = \frac{\Delta^L f_{t+j}}{N_t^2 \Delta^L \sinh(N_t x_{t+j} + A_t)} \, , \; j=0,1,\ldots,k-1 \tag{6.4.2}$$

(b) The hyperbolic functions to be solved for the parameters N_t and A_t are given as follows:

$$R_1(N_t,A_t) = \Delta^L f_{t+1}.\Delta^L \sinh(N_t x_t + A_t) - \Delta^L f_t.\Delta^L \sinh(N_t x_{t+1} + A_t) = 0, \tag{6.4.3}$$

$$R_2(N_t,A_t) = \Delta^L f_{t+2}.\Delta^L \sinh(N_t x_{t+1} + A_t) - \Delta^L f_{t+1}.\Delta^L \sinh(N_t x_{t+2} + A_t) = 0 \tag{6.4.4}$$

and

$$R_3(N_t,A_t) = \Delta^L f_t.\Delta^L \sinh(N_t x_{t+2} + A_t) - \Delta^L f_{t+2}.\Delta^L \sinh(N_t x_t + A_t) = 0 \quad . \tag{6.4.5}$$

As before, we solve any two suitable pairs of the equations (6.4.3) to (6.4.5) for the parameters N_t and A_t.

The limiting values of these parameters are denoted by N_t^* and A_t^*.

(c) The initial estimates $N_0^{[0]}$ and $A_0^{[0]}$ used in the Newton iteration to generate N_t^* and A_t^* are given either as:

$$N_0^{[0]} = \left[\frac{\Delta^4 y_0}{\Delta^2 y_0}\right]^{\frac{1}{2}} , \tag{6.4.6}$$

and

$$A_0^{[0]} = \coth^{-1}\left[\frac{\Delta^3 y_0}{N_0^{[0]} . \Delta^2 y_0}\right] - N_0^{[0]} .a; \tag{6.4.7}$$

or

$$N_0^{[0]} = \left[\frac{\Delta^5 y_0}{\Delta^3 y_0}\right]^{\frac{1}{2}} , \tag{6.4.8}$$

and

$$A_0^{[0]} = \tanh^{-1}\left[\frac{\Delta^4 y_0}{N_0^{[0]} . \Delta^3 y_0}\right] - N_0^{[0]} .a . \tag{6.4.9}$$

Equations (6.4.6) to (6.4.9) are obtained by replacing the higher order derivatives of f(x,y) in equation (4.8.2) to (4.8.4) by the equivalent higher forward differences.

(d) The final integration formula for the case L=1 and k=4 is given as follows:

$$y_{t+k} = - \sum_{j=0}^{k-1} \alpha_j y_{t+j} + h^2 \sum_{j=0}^{k-1} \beta_j f_{t+j}$$

$$+ \frac{(f_{t+3} - f_{t+2})}{N_t^{*2} \left[\sinh(N_t^* x_{t+3} + A_t^*) - \sinh(N_t^* x_{t+2} + A_t^*)\right]} \times$$

$$\left[\sum_{j=0}^{k} \alpha_j \sinh(N_t^* x_{t+j} + A_t^*) - N_t^{*2} h^2 \sum_{j=0}^{k-1} \beta_j \sinh(N_t^* x_{t+j} + A_t^*)\right] . \tag{6.4.10}$$

By following the same procedure as in section (6.3) we can readily establish that the linear multistep formula given by equation (6.4.10) is consistent and zero stable and hence convergent.

6.5 APPLICATIONS AND NUMERICAL RESULTS

We consider the Rayleigh's oscillator equation given by (1.5.2) for the case k=0 and n=1. This yields the system,

$$y'' = -y \qquad (6.5.1)$$

The numerical solution to the problem (6.5.1) was obtained in the range $0 \leq x \leq \pi$ with three sets of initial conditions:—

(a) The first set of initial conditions are given as follows,

$$y(0) = 0 \ ,$$

$$\text{and} \qquad y'(0) = 1 \ . \qquad (6.5.2)$$

The problem (6.5.1) with the initial conditions given by equation (6.5.2) has theoretical solution

$$y(x) = \sin(x) \ . \qquad (6.5.3)$$

Details of numerical results are given in table (6.5.1a).

(b) The second set of initial conditions are specified as:

$$y(0) = 1 \ ,$$

$$y'(0) = 0 \ . \qquad (6.5.4)$$

With these initial values, the problem (6.5.1) has the theoretical solution

$$y(x) = \cos x \qquad (6.5.5)$$

The details of the numerical results are available in table (6.5.1b).

(c) Finally, we assign the initial values:

$$y(0) = 1,$$

$$y'(0) = 1 \ , \qquad (6.5.6)$$

to the problem (6.5.1). This yields a theoretical solution

$$y(x) = \sin x + \cos x.$$

The details of the numerical solution are given by table (6.5.1c).

TABLE (6.5.1a)

$N_0^{[0]} = 0.98659652$

$A_0^{[0]} = 0.13617502$

t	NO. OF NEWTON ITERATIONS	X_t	N_t	A_t	Y_t	$10^8 x T_{t+1}$
0	6	0.00000000	0.9999999	0.0000000	0.0000000	0.00000
1	1	0.15707963	0.9999999	0.0000001	0.15643446	0.67337
2	1	0.31415926	1.0000000	0.0000001	0.30901699	0.57362
3	1	0.47123889	1.0000000	0.0000000	0.45399050	0.48390
4	1	0.62831852	1.0000000	0.0000000	0.58778525	0.26624
5	1	0.78539815	1.0000000	0.0000000	0.70710678	0.27448
6	1	0.94247778	1.0000000	0.0000000	0.80901699	0.28195
7	1	1.09955741	1.0000000	0.0000000	0.89100652	0.28357
8	1	1.25663704	1.0000000	0.0000000	0.95105652	0.28230
9	1	1.41371667	1.0000000	0.0000001	0.98768834	0.27820
10	1	1.57079630	1.0000000	0.0000000	1.00000001	0.26921
11	1	1.72787593	1.0000000	0.0000000	0.98768835	0.25807
12	1	1.88495556	1.0000000	0.0000001	0.95105653	0.24128
13	1	2.04203519	1.0000000	0.0000000	0.89100654	0.22278
14	1	2.19911482	1.0000000	0.0000001	0.80901702	0.19748
15	1	2.35619445	1.0000000	0.0000000	0.70710681	0.17049
16	1	2.51327408	1.0000000	0.0000000	0.58778529	0.13335
17	-	2.67035371	-	-	0.45399054	0.08782
18	-	2.82743334	-	-	0.30901704	0.02863
19	-	2.98451297	-	-	0.15643451	0.03885
20	-	3.14159265	-	-	0.00000000	0.13890

TABLE (6.5.1b)

$N_0^{[0]} = 0.98659652$

$A_0^{[0]} = 1.72836577$

t	NO. OF NEWTON ITERATIONS	X_t	N_t	A_t	Y_t	$10^8 x T_{t+1}$
0	4	0.00000000	0.9999980	1.5707963	1.00000000	0.00000
1	2	0.15707963	1.0000008	1.5707963	0.98768834	0.99420
2	2	0.31415926	0.9999997	1.5707964	0.95105651	0.50121
3	1	0.47123889	1.0000001	1.5707963	0.89100652	0.75607
4	1	0.62831852	1.0000000	1.5707964	0.80901699	0.79637
5	1	0.78539815	1.0000000	1.5707963	0.70710677	1.01652
6	1	0.94247778	1.0000000	1.5707964	0.58778525	1.24184
7	1	1.09955741	1.0000000	1.5707964	0.45399049	1.48623
8	1	1.25663704	1.0000000	1.5707964	0.30901699	1.75310
9	1	1.41371667	1.0000000	1.5707963	0.15643446	2.05377
10	1	1.57079630	1.0000000	1.5707963	0.00000000	2.39258
11	1	1.72787593	1.0000000	1.5707964	-0.15643446	2.02908
12	1	1.88495556	1.0000000	1.5707963	-0.30901699	1.71391
13	1	2.04203519	1.0000000	1.5707963	-0.45399049	1.43243
14	1	2.19911482	1.0000000	1.5707964	-0.58778524	1.17677
15	1	2.35619445	1.0000000	1.5707963	-0.70710678	0.94322
16	1	2.51327408	1.0000000	1.5707964	-0.80901698	0.71995
17	-	2.67035371	-	-	-0.89100651	0.51328
18	-	2.82743334	-	-	-0.95105651	0.31288
19	-	2.98451297	-	-	-0.98768834	0.12043
20	-	3.14159265	-	-	-1.00000000	0.70577

TABLE (6.5.1c)

$N_0^{[0]} = 1.05782428$

$A_0^{[0]} = 0.94022931$

t	NO. OF NEWTON ITERATIONS	X_t	N_t	A_t	Y_t	$10^8 x T_{t+1}$
0	5	0.00000000	1.0000009	0.7853975	1.00000000	0.00000
1	2	0.15707963	0.9999993	0.7853987	1.14412281	0.30609
2	2	0.31414926	1.0000006	0.7853977	1.26007351	0.89498
3	2	0.47123889	0.9999992	0.7853988	1.34499703	0.58580
4	1	0.62831852	0.9999996	0.7853985	1.39680226	0.51850
5	1	0.78539815	1.0000001	0.7853981	1.41421358	0.62325
6	1	0.94247778	1.0000000	0.7853982	1.39680227	0.73099
7	1	1.09955741	1.0000000	0.7853981	1.34499705	0.82967
8	1	1.25663704	1.0000000	0.7853982	1.26007355	0.92846
9	1	1.41371667	1.0000000	0.7853982	1.14412285	1.02346
10	1	1.57079630	1.0000001	0.7853981	1.00000005	1.11831
11	1	1.72787593	1.0000000	0.7853982	0.83125393	1.21421
12	1	1.88495556	1.0000000	0.7853981	0.64203958	1.30760
13	1	2.04203519	1.0000000	0.7853982	0.43701609	1.40885
14	1	2.19911482	1.0000000	0.7853981	0.22123181	1.51464
15	1	2.35619445	1.0000000	0.7853981	0.00000007	1.62612
16	1	2.51327408	1.0000000	0.7853982	-0.22123167	1.11815
17	-	2.67035371	-	-	-0.43701595	0.73797
18	-	2.82743334	-	-	-0.64203945	0.45064
19	-	2.98451297	-	-	-0.83125381	0.21892
20	-	3.14159265	-	-	-1.00000000	0.02474

With the view to compare and contrast the new numerical integration schemes developed in chapters IV,V and VI with some standard existing schemes, test runs were carried out on the problem (6.5.1) with the initial conditions specified by (6.5.2).

Apart from the new schemes, the problem was also solved using the following standard numerical integration schemes:

(a) Gragg-Bulirsch-Stoer algorithm as discussed in chapter III.

(b) Gautschi's multistep scheme as discussed in chapter II and

(c) Krogh's variable order Adam's scheme (the Numerical Algorithm Group's version).

The details of the numerical results are given in tables (6.5.1d) to (6.5.1e).

Apart from Krogh's method, all the schemes maintained an accuracy of 10^{-8} with uniform integration mesh size of $h=\frac{\pi}{20}$. In fact, the one step scheme still maintained the same degree of accuracy with a uniform mesh-size of $h=\frac{\pi}{10}$ as shown in table (6.5.1g).

With a uniform mesh size of $h=\frac{\pi}{20}$, Gautschi's scheme of trigonometric order one produced a smaller truncation error than the variable order Gragg-Bulirsch-Stoer algorithm of order in $(6 \leq m \leq 8)$, The linear multistep method proposed in chapter V produced better results than Gautschi's scheme whilst in turn, the special multistep scheme of chapter VI has even smaller truncation errors than the scheme proposed in chapter V. The one step scheme proposed in chapter IV provided the most accurate results as the oscillatory parameters N_t and A_t are accurately determined at each step of the integration procedure. The degree of accuracy of the linear multistep formulae developed in chapters V and VI is constrained by the fact that the parameters N_t and A_t are determined to a limited degree of accuracy.

TABLE (6.5.1d)

KROGH'S VARIABLE ORDER ADAMS

INITIAL STEPSIZE H=0.15707963

H	X	Y	$10^8 x T_{t+1}$
0.01963495	0.00000000	0.00000000	0.00000
0.03926991	0.31415926	0.30901699	0.00056
0.07853982	0.62831852	0.58778524	0.00046
0.07853982	0.94247778	0.80901698	0.00121
0.07853982	1.25663704	0.95105651	0.00075
0.07853982	1.57079630	1.00000000	0.00000
0.07853982	1.88495556	0.95105653	0.00075
0.07853982	2.19911482	0.80901702	0.00281
0.15707963	2.51327408	0.58778529	0.00560
0.15707963	2.82743334	0.30901704	0.00500
0.15707963	3.14159265	0.00000000	0.02288

TABLE (6.5.1e)

GRAGG-BULIRSCH-STOER

ORDER OF EXTRAPOLATION	H	X	Y	$10^8 x T_{t+1}$
6	0.15707963	0.00000000	0.00000000	0.00000
8	0.15707963	0.15707963	0.15643446	0.16862
8	0.15707963	0.31415926	0.30901699	0.23123
8	0.15707963	0.47123889	0.45399050	0.24445
8	0.15707963	0.62831852	0.58778525	0.20713
8	0.15707963	0.78539815	0.7071678	0.36399
8	0.15707963	0.94247778	0.80901699	0.40180
8	0.15707963	1.09955741	0.89100652	0.36360
8	0.15707963	1.25663704	0.95105651	0.25322
8	0.15707963	1.41371667	0.98768834	0.25843
6	0.15707963	1.57079630	1.00000000	0.00146
8	0.157079 3	1.72787593	0.98768833	0.51320
8	0.15707963	1.88495556	0.95105651	0.92373
8	0.15707963	2.04203519	0.89100651	1.42056
8	0.15707963	2.19911482	0.80901698	2.01465
8	0.15707963	2.35619445	0.70710676	2.71329
8	0.15707963	2.51327408	0.58778523	3.28104
8	0.15707963	2.67035371	0.45399048	3.95201
8	0.15707963	2.82743334	0.30901698	4.74154
8	0.15707963	2.98451297	0.15643445	5.67513
8	0.15707963	3.14159265	0.00000000	6.89314

TABLE (6.5.1f)

GAUTSCHI'S SCHEME

H	X	Y	$10^8 x T_{t+1}$
0.15707963	0.00000000	0.00000000	0.00000
0.15707963	0.31415926	0.30901699	0.34879
0.15707963	0.62831852	0.58778525	0.56639
0.15707963	0.94247778	0.80901700	0.59647
0.15707963	1.25663704	0.95105652	0.45385
0.15707963	1.57079630	1.00000000	0.13606
0.15707963	1.88495556	0.95105652	0.37628
0.15707963	2.19911482	0.80901700	1.12255
0.15707963	2.51327408	0.58778525	2.17346
0.15707963	2.82743334	0.30901699	3.65822
0.15707963	3.14159265	0.00000000	5.85113

TABLE (6.5.1g)

ONE STEP SCHEME (CHAPTER IV)

ONE STEP ORDER 4

H	X	Y	$10^{8} x T_{t+1}$
0.31415926	0.00000000	0.00000000	0.00000
0.31415926	0.31415926	0.30901699	0.00000
0.31415926	0.62831852	0.58778524	0.00092
0.31415926	0.94247778	0.80901698	0.00161
0.31415926	1.25663704	0.95105651	0.00261
0.31415926	1.57079630	1.00000000	0.00363
0.31415926	1.88495556	0.95105653	0.00336
0.31415926	2.19911482	0.80901702	0.00362
0.31415926	2.51327408	0.58778529	0.00367
0.31415926	2.82743334	0.30901704	0.00111
0.31415926	3.14159265	0.00000000	0.00531

TABLE (6.5.1h)

LINEAR MULTISTEP SCHEME (CHAPTER V)

H	X	Y	$10^8 x T_{t+1}$
0.15707963	0.00000000	0.00000000	0.00000
0.15707963	0.31415926	0.30901699	0.57362
0.15707963	0.62831852	0.58778524	0.19155
0.15707963	0.94247778	0.80901698	0.05992
0.15707963	1.25663704	0.95105651	0.02312
0.15707963	1.57079630	0.99999999	0.71159
0.15707963	1.88495556	0.95105652	0.42551
0.15707963	2.19911482	0.80901702	0.43438
0.15707963	2.51327408	0.58778526	1.44622
0.15707963	2.82743334	0.30901702	1.19115
0.15707963	3.14159265	0.00000000	4.08836

TABLE (6.5.1i)

SPECIAL MULTISTEP SCHEME (CHAPTER VI)

H	X	Y	$10^{8}xT_{t+1}$
0.15707963	0.00000000	0.00000000	0.00000
0.15707963	0.31415926	0.30901699	0.57362
0.15707963	0.62831852	0.58778525	0.26624
0.15707963	0.94247778	0.80901699	0.28195
0.15707963	1.25663704	0.95105651	0.28230
0.15707963	1.57079630	1.00000001	0.26921
0.15707963	1.88495556	0.95105653	0.24128
0.15707963	2.19911482	0.80901702	0.19748
0.15707963	2.51327408	0.58778529	0.13335
0.15707963	2.82743334	0.30901704	0.02863
0.15707963	3.14159265	0.00000000	0.13890

SUMMARY OF RESULTS

TABLE (6.5.1j)

X	KROGH'S METHOD H	KROGH'S METHOD $10^8 x T_{t+1}$	GRAGG-BULIRSCH-STOER H= 0.15707963 $6 \leq M \leq 8$ $10^8 x T_{t+1}$	GAUTSCHI H= 0.15707963 $10^8 x T_{t+1}$	ONE STEP SCHEME OF ORDER 4 CHAPTER IV H= 0.314159265 $10^8 x T_{t+1}$	MULTISTEP SCHEME CHAPTER V H=0.15707963 $10^8 x T_{t+1}$	MULTISTEP SCHEME CHAPTER VI H=0.15707963 $10^8 x T_{t+1}$
0.00000000	0.01963495	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.31415926	0.03926991	0.00056	0.23123	0.34879	0.00036	0.57362	0.57362
0.62831852	0.07853982	0.00046	0.20713	0.56639	0.00092	0.19155	0.26624
0.94247778	0.07853982	0.00121	0.40180	0.59647	0.00161	0.05992	0.28195
1.25663704	0.07853982	0.00075	0.25322	0.45385	0.00261	0.02312	0.28230
1.57079630	0.07853982	0.00000	0.00146	0.13606	0.00363	0.71159	0.26921
1.88495556	0.07853982	0.00075	0.92373	0.37628	0.00336	0.42551	0.24128
2.19911482	0.07853982	0.00281	2.01465	1.12255	0.00362	0.43438	0.19748
2.51327408	0.15707963	0.00560	3.28104	2.17346	0.00367	0.44622	0.13335
2.82743334	0.15707963	0.00500	4.74154	3.65822	0.00111	1.19115	0.02863
3.14159265	0.15707963	0.02288	6.89314	5.85113	0.00531	4.08836	0.13890

6.6 CONCLUDING REMARKS

The new one step integration scheme proposed in chapter IV is particularly accurate for oscillatory systems of both linear and nonlinear form. In cases where accuracy is essential and desirable we highly recommend this scheme. The fact that the scheme is capable of using relatively larger integration stepsizes than the other existing numerical integration formulae is a great asset. For linear oscillatory systems, both the linear multistep schemes proposed in chapters V and VI are competitive with the standard existing integration procedures. For the second order oscillatory systems in which the first derivative does not appear explicitly, the integration formulae developed in chapter VI is very efficient and gives more accurate results than the integration formulae developed in chapter V.

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