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NUMERICAL TREATMENT OF SINGULAR AND DISCONTINUOUS INITIAL VALUE PROBLEMS.

BY

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M. TECH/96/0033

A MASTER'S DEGREE PROJECT SUBMITTED TO THE DEPARTMENT OF MATHEMATICS AND COMPUTER SCIENCE, FEDERAL UNIVERSITY OF TECHNOLOGY, MINNA. IN PARTIAL FULFILMENT OF THE REQUIREMENT FOR THE AWARD OF MASTERS OF TECHNOLOGY (M. TECH) MATHEMATICS.

NOVEMBER, 1998.

Certification

This is to certify that this research project has been read and approved as meeting the requirements of the Department of Mathematics and Computer Science, Federal University of Technology, (FUT) Minna, for the award of Master of Technology in Mathematics.

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ACKNOWLEDGEMENT

I am very much indebted to the Department of Mathematics and Computer Science, Federal University of Technology (FUT), Minna for giving me the opportunity to carry out this project. I am particularly grateful to my mentor and Supervisor, Professor K.R. Adeboye for his intellectual guidance. I am debted to Professor Adeboye for taking the time to read through the whole script. His useful comments and constructive criticisms and suggestions have made this research work possible.

I am grateful to the entire staff of the Department of Mathematics and Computer Science, FUT, Minna, for their co-operation and assistance.

I am also indebted to Dr. Francis N. Gana for his encouragement and assistance.

Were I to acknowledge the whole extent of my indebtedness to others, I should transfer to this point the bibliography which appears as an appendix. But passing over those to whom I am indebted through their published work, I feel it my duty, as it is my previlege, to mention two names in particular. To Prof. S.O. Fatunla I owe my introduction to the subject; to Professor K.R. Adeboye my initiation into research and many acts of kind encouragement.

I am grateful to Mal. Ismaila M. Egbako, Mr. Gabriel R.S. and many of friends whose names do not appear here for their moral support.

Above all, I give glory to Almighty Allah for His guidance, wisdom and protection.

ABSTRACT

This research project was conceived within the framework of the philosophy that there are some initial value problems in which some components of the solution contain discontinuities.

In this attempt some topical review of earlier treatments of singular and discontinuous initial value problems were made.

A two-step numerical integrator is presented based on the inverse polynomial methods. The numerical results for the integrator are contrasted with some earlier works. The integrator converges rapidly when used to solve initial value problems with discontinuities / singularities in the solutions. The integrator is zero-stable and is well suited for singular and discontinuous initial value problems.

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CHAPTER ONE

General Introduction and Basic Mathematical Ideas

1.1 Historical Background

A branch of mathematics which has enjoyed almost three centuries of rigorous life and whose early history tends more and more to be masked by the density of its later growth is Differential Equation. Yet our hazy knowledge of the birth and infancy of the science of differential equation condenses upon a remarkable date, the 11th November, 1675, when Leibniz first set down on paper the equation

$$\int y\, dy = \tfrac{1}{2}y^2,$$

thereby not merely solving a simple differential equation, which was in itself a trivial matter, but what was an act of great moment, forging a powerful tool, the integral sign.

The early history of the infinitesimal calculus abounds in instances of problems solved through the agency of what were virtually differential equations; it is even true to say that the problem of integration which may be regarded as the solution of the simplest of all types of differential equations, was a practical problem. Particular cases of the inverse problem of tangents, that is the problem of determining a curve whose tangents are subjected to a particular law, were successfully dealt with before the invention of the calculus.

But the historical value of science depends not upon the number of particular phenomena it can present but rather upon the power it has of coordinating diverse facts and subjecting them to one simple code. That was what Newton considered when he classified differential equations of the first order, that time known as fluxional equations, into three classes.

The first clss is composed of those equations in which two fluxions x' and y'and one fluent x or y, are related. For example

$$y' = f(x) \quad \text{or} \quad \frac{dy}{dx} = f(x)$$

and $$y' = f(y) \quad \text{or} \quad \frac{dy}{dx} = f(y)$$

The second class composed of those equations which involve two fluxions and two fluents. That is

$$y' = f(x,y) \text{ or } \frac{dy}{dx} = f(x,y)\cdot$$

The third class is made up of equations which involve more than two fluxions; these are known as partial differential equation.

By the end of the seventeenth century practically all the known elementary methods of solving differential equations of the first order had been brought to light. The problem of determing the orthogonal trajectories of a one-parameter family of curves was solved by John Bernoulli in 1698; the problem of oblique trajectories presented no further difficulties. In early years of eighteenth century a number of problems which led to differential equations of the second or third orders were discovered. In 1696 James Bernoulli formulated the isoperimetric problem, or the problem of determing curves of a given perimeter which shall under given conditions , enclose a maximum area. Some

DEDICATION

This work is dedicated to my beloved wife, Hajara A.A. and my children Mohammed, Yakubu and Salamatu Ahmed.

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five years later he published equation of the third order. The problem of trajectories in a general sense and in particular trajectories defined by the knowledge point gave rise to differential equations of the second order. Thus for example, John Bernoulli, discussed an equation which would be written as

$$\frac{d^2y}{dx^2} = \frac{2y}{x^2} ;$$

and stated that it gave rise to three types of curves, parabola, hyperbola and a class of curves of third order.

Numerical Methods of Ordinary Differential Equations

Of all the ordinary differential equations of the first order, only certain very special types admit of explicit integration, and when an equation which is not of one or other of these types arises in a practical problem the investigator has to fall back upon purely numerical methods of approximating the required solution.

Consider the differential equation

$$\frac{dy}{dx} = f(x,y) \quad \text{or} \quad y' = f(x,y).$$

It will be supposed that the initial value (x_o, y_o) is not singular with respect to the equation, and that a solution exists which can be developed in Taylor series, thus:

$$K = hy' + \frac{h^2}{2!}y'' + \frac{h^3}{3!}y''' + \frac{h^4}{4!}y^{iv} + \ldots.$$

where $h = x - x_o$, and $K = y - y_o$ and h is sufficiently small.

Now the coefficients in the Taylor series may be calculated as follows:

$$y' = f(x,y),$$

$$y'' = \frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y},$$

$$y''' = \frac{\partial^2 f}{\partial x^2} + \frac{2f\partial^2 f}{\partial x \partial y} + \frac{f^2\,\partial^2 f}{\partial y^2} + \left(\frac{\partial f}{\partial x} + f\frac{\partial f}{\partial y}\right)\frac{\partial f}{\partial y},$$

and so on ....

but the increasing complexity of these expressions renders the process impracticable. The actual method adopted in practice is Runge's method which is an adaptation of Gauss' method of numerical integration. Four numbers K_1, K_2, K_3, K_4 are defined as follows:

$$K_1 = hf(x_0\ ,\ y_0\ )$$

$$K_2 = hf(x_0 + \alpha h,\quad y_0 + \beta K_1)$$

$$K_3 = hf(x_0 + \alpha_1 h,\ y_0 + \beta_1 k_1 + \mu_2 k_2)$$

$$K_4 = hf(x_0 + \alpha_2 h,\quad y_0 + \beta_2 k_1 + \mu_2 k_2 + \delta_2 k_3)$$

where the nine constants α, β,... δ_2, and four weights R_1, R_2, R_3 R_4 are to be determined so that the expression

$R_1K_1 + R_2K_2 + R_3K_3 + R_4K_4$ agrees with the Taylor series up to and including the term in h^4.

The method above can be extended to systems of any number of equations of the first order, and therefore to equations of order higher than the first. For a system of two equations.

$$\frac{dy}{dx} = f(x,y,z), \quad \frac{dz}{dx} = g(x,y,z)$$

if the initial values are that

$y = y_0$, $z = z_0$ when $x = x_0$, then Runge's method for the increment K and L which y_0 and z_0 receive when x_0 is increased by h are

$$K_1 = hf(x_0,\ y_0,\ z_0),$$
$$K_2 = hf(x_0 + \tfrac{1}{2}h,\ y_0 + \tfrac{1}{2}K_0,\ z_0 + \tfrac{1}{2}L_1)$$
$$K_3 = hf(x_0 + \tfrac{1}{2}h,\ y_0 + \tfrac{1}{2}k_2,\ z_0 + \tfrac{1}{2}L_2)$$
$$K_4 = hf(x_0 + \tfrac{1}{2}h,\ y_0 + k_3,\ y_0 + L_3)$$

$$L_1 = hg(x_0,\ y_0,\ z_0)$$
$$L_2 = hg(x_0 + \tfrac{1}{2}h,\ y_0 + \tfrac{1}{2}k_1,\ z_0 + \tfrac{1}{2}L_1)$$
$$L_3 = hg(x_0, + \tfrac{1}{2}h,\ y_0 + \tfrac{1}{2}k_2,\ z_0 + \tfrac{1}{2}L_2)$$
$$L_4 = hg(x_0 + h,\ y_0 + k_3,\ z_0 + L_3)$$

$$K = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_3)$$

$$L = \frac{1}{6}(L_1 + 2L_2 + 2L_3 + L_4).$$

In its original form the method discussed above is due to Runge; later modifications are due, among others to Kutta. Hence the method is later called Runge-Kutta method.

1.1.2 Singular Solutions

Singular solutions were discovered in a rather surprising manner. Brook Taylor set out to discover the solution of a certain differential equation which, in modern symbolism, would be written as:

$$(1 + x^2)^2 \left(\frac{dy}{dx}\right)^2 = 4y^3 - 4y^2$$

He substituted $y = u^{\lambda} v^{\mu}$, where

u and v were new variables and λ and μ contants to be determined, and so transformed the equation into:

$$(1 + x^2)^2 \left(\mu u \frac{dv}{dx} + \lambda v \frac{du}{dx}\right)^2 = 4u^{\lambda+2} v^{\mu+2} - 4u^2 v^2$$

In this equation there are three elements whose choice is unrestricted, namely λ, μ and v;u is then the new dependent variable

Firstly let

$$v = 1 + x^2$$

then, dividing through by $(1 + x^2)^2$, the equation becomes

$$\left(2\mu x u + \lambda v \frac{dy}{dx}\right)^2 = 4u^{\lambda+2} v^{\mu} - 4u^2.$$

Now let $\lambda = -2$, $\mu = 1$ and the equation reduces to

$$\left(2xu - 2v \frac{du}{dx}\right)^2 = 4v - 4u^2,$$

that is

$$(1 + x^2)\, u^2 - 2xuv \frac{du}{dx} + v^2 \left(\frac{du}{dx}\right)^2 = v$$

or, since $v = 1 + x^2$,

$$u^2 - 2xu\frac{du}{dx} + v\left(\frac{du}{dx}\right)^2 = 1$$

Now, if this equation is differentiated with respect to x, the derived equation is

$$2\frac{d^2u}{dx^2}\left(v\frac{du}{dx} - xu\right) = 0$$

and breaks up into two equations namely

$$\frac{d^2u}{dx^2} = 0, \quad v\frac{du}{dx} - xu = 0$$

The first gives $\frac{d^2u}{dx^2} = a$,

where a is constant; when this value is substituted in the differential equation for u, the later degenerates into the algebraic equation; $(u - ax)^2 = 1-a^2$.

The general solution of the original equation is therefore

$$y = \frac{v}{u^2} = \frac{1 + x^2}{(ax + \sqrt{1-a^2})^2}.$$

The second equation,

$$v\frac{du}{dx} - xu = 0,$$

taken in conjunction with

$$u^2 - 2xu\frac{du}{dx} + v\left(\frac{du}{dx}\right)^2 = 1$$

gives $1 = u^2 - \frac{2x^2u^2}{v} + \frac{x^2u^2}{v}$

Or $v = u^2(v - x^2) = u^2$

$\therefore\ y = \frac{v}{u^2} = 1$

This is truly a solution of the original equation, but it cannot be derived from the general solution by attributing a particular value to a. It is therefore a singular solution.

1.2 Definitions

In this project the following definitions shall be adopted.

1.2.1 Differential Equation

A differential equation is a relationship between the differential dx and dy of two vairables x and y. Such relationship in general explicitly involves the variable x and y together with other sumbols a, b, c.... which represent constants. In other words, differential equations can be understood to include any algebraical or transcendental equalities which involve either differentials or differential coefficients. But it should be understood that differential equation is not an identity.

1.2.2 Initial Value Problems

The general form of the ordinary differential equation can be put in the form

$$L[Y] = r \qquad \text{\_\_\_\_\_\_\_\_\_\_} \quad (1.2.1)$$

where L is a differential operator and r is a given function of the independent variable x. A linear differential equation of order n can be expressed in the form

$$L[Y] = \sum_{p=v}^{n} f_p(x) y^p(x) = r(x) \qquad \text{\_\_\_\_\_\_\_\_\_\_} \quad (1.2.2)$$

in which $f_p(x)$ are known functions. The general non linear differential equation of order n can be written as

$$F[x,y,y',y''\ldots y^{(n-1)}, y^{(n)}] = 0 \quad \text{\_\_\_\_\_\_(1.2.3)}$$

$$\text{Or} \quad y^{(n)}(x) = f[x,y,y',y''\ldots y^{(n-1)}] \quad \text{\_\_\_\_\_\_(1.2.4)}$$

where $x \in [a,b]$

The general solution of the nth order ordinary differential equation contains n independent arbitrary constants. In order to determine the arbitrary constants in the general solution if the n conditions are prescribed at one point, these are the initial conditions. The differential equation together with an initial conditions is called the initial value problem.. Thus, the nth order initial value problem can be expressed as

$$y^n(x) = f(x,y,y',y''\ldots y^{(n-1)})$$

$$y^p(x_o) = y_o{}^{(p)}, \qquad p = 0,\ 1,\ 2\ \ldots\ldots\ n - 1$$

If the n conditions are prescribed at more than one point, these are called boundary conditions. The differential equation together with boundary condtions is called boundary value problem.

1.2.3 Numerical Methods

Consider the differential equation

$$y' = f(x,y),\ y(x_0) = y_0 \quad \text{———} \quad (1.2.6)$$

$$x \in [a,b]$$

The numerical methods for the solution of the differential equation (1.2.6) are the algorithms which will produce a table of approximate values y(x) at certain equally spaced points called, grid or mesh points along the x coordinate. Each mesh point in terms of the previous point is determined by the relationship

$$x_{n+1} = x_n + h, \quad n = 0,1,2 \ldots\ldots N - 1$$

$$x_0 = a, x_N = b$$

where h is called the step length. Alternatively, we may write

$$x_n = x_o + nh, \quad n = 1,2 \ldots N$$

The numerical methods for finding solution of the initial value problem of equation (1.2.6) may be broadly classified into the following two types:

(i) Singlestep Methods: These methods enable us to find approximation to the true solution y(x) at x_{n+1} if y_n, y'_n and h are known.

(ii) Multistep Methods: These methods use recurrence relations, which express the function value y(x) at x_{n+1} in terms of the function values y(x) and derivative values $y'(x)$ at x_{n+1} and at previous mesh points.

1.3 The Linear Multistep Methods

Consider the initial value problem for a first-order differential equation:

$$y' = f(x,y), \quad y(a) = A \quad \text{\_\_\_\_\_\_\_\_} \quad (1.3.1)$$

We seek a solution in the interval $a \le x \le b$, where a and b are finite and we assume that $f(x,y)$ satisfied the following conditions:

(i) $f(x,y)$ is a real function

(ii) $f(x,y)$ is defined and continuous in the interval $x \in [a,b]$, $y \in (-\infty, \infty)$

(iii) there exists a constant L such that for any $x \in [a,b]$ and for any two numbers y_1 and y_2

$$|f(x,y_1)-f(x,y_2)| \le L|y_1-y_2|,$$

where L is called Lipschitz constant.

Then for any y_0 the initial value problem (1.3.1) has a unique solution $y(x)$ for $x \in [a,b]$. Consider the sequence of points $\{x_n\}$ defined by $x_n = a + nh$, $n = 0,1,2.....$, where h is the step length. An important property of the majority of computational methods of the solution (1.3.1) is that of discretization; that is, we seek an approximate solution, not on the continuous interval $a \le x \le b$, but on the discrete point $\{x_n\}$, $n = 0,1,2....,\frac{b-a}{h}\}$. Let y_n be an approximation to the theoretical solution at x_n, that is to $y(x_n)$ and let $f_n = f(x_n,y_n)$. A computational method to determine the sequence $\{y_n\}$ which takes the form of a linear relationship between y_{n-j}, f_{n+j}, $j=0,1,2,....k$, is called a linear multistep method of step number k, or a linear k-step method.

The general linear multistep method may, therefore, be written as

$$\sum_{j=0}^{k}\alpha_j y_{n+j}=h\sum\beta_j f_{n+j} \quad \text{———} \quad (1.3.2)$$

where α_j and β_j are constants; we assume that $\alpha_0\neq0$ and that not both α_0 and β_0 are zero.

The problem of determining the solution y(x) of the initial value problem (1.3.1) can be replaced by that of finding a sequence $\{y_n\}$, which satisfies the difference equation (1.3.2). Such equations are not easy to handle. In order to compute the sequence $\{y_n\}$ numerically, we must have a set of some starting values $y_o, y_1, \ldots y_{k-1}$. In the case of one-step method, only one such value, y_o, is needed and we usually choose $y_o = A$.

The difference method (1.3.2) is said to be explicit if $\beta_k=0$, $\alpha_k\neq0$ and implicit if $\beta_k\neq0$ and $\alpha_k\neq0$ for an explicit method, (1.3.2) yields the current value y_{n+k} directly in terms of y_{n+j}, f_{n+j} j=0,1....k-1. While an implicit method calls for the solution at each stage of the computation of the equation.

$$y_{n+k} = h\beta_k f(x_{n+k}, y_{n+k}) + g, \quad \text{———} \quad (1.3.3)$$

where g is a known function of the previously calculated values y_{n+j}, f_{n+j}, n =0,1... k-1.

We finally turn to problem of determining the coefficients α_j, β_j which appeared in (1.3.2). Any specific linear multistep method may be derived in a number of different ways. We shall consider some different approaches which throw light on the nature of the approximation involved.

1.3.1 Derivation Through Taylor Expansion

Consider the Taylor expansion for $y(x_n+h)$ about x_n.

$$y(x_n + h) = y(x_n)+hy'(x_n)+\frac{h^2}{2!}y''(x_n)+\frac{h^3}{3!}y'''(x_n) + \ldots$$

Truncating this expansion after two terms and subtitute for $y'(x)$ from the differential equation (1.3.1), we have

$$y(x_n + h) \cong y(x_n) + hf[x_n, y(x_n)] \qquad \text{———} \qquad (1.3.4)$$

Equation (1.3.4) gives an approximate relation between exact values of the solution of (1.3.1). It is also a relationship between the exact solution and approximate solution of (1.3.1). If we replace $y(x_n)$, $y(x_n+h)$ by y_n, y_{n+1} respectively to give

$$y_{n+1} = y_n+hf_n \qquad \text{———} \qquad (1.3.5)$$

This is an explicit linear one-step method known as Euler's rule. The error associated with it is given in the expression

$$\frac{h^2}{2!} y''(x_n) + \frac{h^3}{3!} y'''(x_n) + \ldots\ldots$$

Now, if we consider Taylor expansions for $y(x_n+h)$ and $y(x_n-h)$ about x_n:

$$y(x_n+h) = y(x_n)+hy'(x_n)+\frac{h^2}{2!}y''(x_n)+\frac{h^3}{3!}y'''(x_n)+\ldots$$

$$y(x_n-h) = y(x_n)- hy'(x_n) +\frac{h^2}{2!}y''(x_n)-\frac{h^3}{3!}y'''(x_n)+\ldots$$

Subtracting, we obtain

$$y(x_n+h) - y(x_n-h) = 2hy'(x_n) + \frac{h^3}{3}y'''(x_n) + \ldots\ldots$$

Using the same argument as above, we obtain a linear multistep method

$$y_{n+1} - y_{n-1} = 2hf_n \quad \text{————} \quad (1.3.6)$$

If we replace n by n+1 in (1.3.6) we get

$$y_{n+2} - y_n = 2hf_{n+1} \quad \text{————} \quad (1.3.7)$$

which is called the Mid-point rule. Its local truncation error is defined by

$$\pm \frac{h^3}{3} y'''(x_n) + \ldots\ldots$$

We can use similar approach to derive any linear multistep method of given specification. Suppose we wish to establish the most accurate one-step implicit method,

$$Y_{n+1} + \alpha_0 y_n \cong h[\beta_1 f_{n+1} + \beta_0 f_n],$$

we write its associated approximate relationship

$$y(x_n+h)+\alpha_0 y(x_n) \cong h[\beta y'(x_n+h) + \beta_0 y'(x_n)] \quad \text{———} \quad (1.3.7)$$

and choose α_0, β_1, β_0 so as to make the aproximation accurate enough. Using the following expansions:

$$y(x_n + h) = y(x_n) + hy'(x_n) + \frac{h^2}{2!}y''(x_n) + \ldots\ldots$$

$$y'(x_n + h) = y'(x_n) + hy''(x_n) + \frac{h^2}{2!}y'''(x_n) + \ldots\ldots$$

Substituting in (1.3.7) and collecting the terms of the left-hand side gives .

$$C_o y(x_n) + C_1 h y'(x_n) + C_2 h^2 y''(x_n) + C_3 h^3 y'''(x_n) + \ldots = 0$$

where $C_o = 1 + \alpha_0$, $C_1 = 1 - (\beta_1 - \beta_0)$, $C_2 = ½ - \beta_1$, $C_3 = \frac{1}{6} - ½\beta_1$

Therefore, to make the approximation in (1.3.7) accurate enough, we choose $\alpha_0 = -1$, $\beta_1 = \beta_0 = ½$ hence $C_3 = -\frac{1}{12}$.

Then the linear multistep is now

$$y_{n+1} - y_n = h/2(f_{n+1} + f_n) \quad \text{——————} \quad (1.3.8)$$

which is called the Trapezoidal rule and its local truncation error is

$$\pm \frac{1}{12} h^3 y'''(x_n) + \ldots\ldots$$

1.3.2. Derivation Through Numerical Integration

Consider:

$$y(x_{n+2}) - y(x_n) \equiv \int_{x_n}^{x_{n+2}} y'(x)\,dx \quad \text{——————} \quad (1.3.8)$$

Using the differential equation (1.2.6) we can replace $y'(x)$ by $f(x,y)$ in the integrand. By using Newton-Gregory forward interpolation formula,

$$P(x) = P(x_n + rh) = f_n + r\,\Delta f_n + \frac{r(r-1)}{2!}\Delta^2 f_n + \ldots\ldots$$

we make the approximation

$$\int_{n}^{x_{n+2}} y'(x)\,dx = \int_{x_n}^{x_{n+2}} P(x)\,dx = \int_{0}^{2} [f_n + r\, f_n + \tfrac{1}{2} r(r-1)\Delta^2 f_n] h\, dr.$$

$$= h(2f_n + 2\,\Delta f_n + \frac{1}{3}\Delta^2 f_n)$$

Expanding Δf_n and $\Delta^2 f_n$ in terms of f_n, f_{n+1}, f_{n+2} and substituting into (1.3.8) we have

$$y_{n+2} - y_n = \frac{h}{3}(f_{n+2} + 4f_{n+1} + f_n) \quad \text{———} \quad (1.3.9)$$

which is Simpson's rule.

Similarly, if we replace (1.3.8) by the identity

$$y(x_{n+2}) - y(x_{n+1}) = \int_{n+1}^{x_{n+2}} y'(x)\, dx$$

and put $y'(x) = P(x)$ as defined above, we obtain

$$y_{n+2} - y_{n+1} = \frac{h}{12}[5f_{n+2} + 8f_{n+1} - f_n] \quad \text{———} \quad (1.3.10)$$

which is a two-step Adams-Moulton methods.

1.3.3 Derivation Through Interpolation

Suppose we wish to derive the implicit two-step method (1.3.9). Let $y(x)$, the solution of (1.3.1), be approximated locally in the range $x_n \le x \le x_{n+2}$ by a polynomial (G(x). If G(x) interpolates the points (x_{n+j}, y_{n+j}), $j = 0,1,2$ and the derivative of G(x) coincides with the prescribed derivative

f_{n+j} for $j = 0,1,2$. Then the conditins imposed on $G(x)$ are thus

$$G(x_{n+j}) = y_{n+j}, \qquad G'(x) = f_{n+j}, \; j = 0,1,2 \text{ —— } (1.3.11).$$

There are six conditions in all. Let $G(x)$ be a polynominal of four degree. That is, $G(x) = ax^4 + bx^3 + cx^2 + dx + e$ Eliminating the five coefficients a, b, c, d, e, between the six equations in (1.3.11) yields the identity

$$y_{n+2} - y_n = \frac{h}{3}(f_{n+2} + 4f_{n+1} + f_n),$$ which is the linear multistep method in (1.3.9).

Suppose $G(x)$ is a polynomial of degree two, namely

$$G(x) = ax^2 + bx + c$$

If we impose the following conditions

$$y_n = G(x_j), \; y_{j+1} = G(x_{j+1}), \; f_j = G'(x_j)$$

and

$$f_{j+1} = G'(x_{j+1})$$

So that $y_j = G(x_j) = ax_j^2 + bx_j + C$

and $y_{j+1} = G(x_{j+1}) = G(x_j + h)$

$$= a(x_j + h)^2 + b(x_j + h) + C$$

$$= a(x^2_j + 2hx_j + h^2) + bx_j + bh + C$$

$$y_{j+1} = ax_j^2 + 2ax_jh + ah^2 + bx_j + bh + C$$

$$f_j = G'(x_j) = 2ax_j + b$$

$$f_{j+1} = G'(x_j + h) = 2a(x_j+h) + b$$

$$= 2ax_j + 2ah + b$$

then $$y_{j+1} - y_j = (ax^2{}_j + bx_j + C) + 2ahx_j + ah_2 + bh - (ax_j + bx_j + C)$$

$$= 2ahx_j + ah^2 + bh$$

$$= h(2ax_j + 2ah + b) - ah^2$$

$$= hf_{j+1} - ah^2$$

$$= hf_{j+1} - \frac{h}{2}(f_{j+1} - f_j) = \frac{h}{2}(f_{j+1} + f_j)$$

$$y_{j+1} - y_j = \frac{h}{2}(f_{j+1} + f_j), \text{ put } j = n$$

we have $$y_{n+1} = y_n + \frac{h}{2}(f_{n+1} + f_n),$$

which is the trapezoidal rule (1.3.8)

1.3.4 Convergence of Linear Multistep Methods

A basic property required for an acceptable linear multistep method is that the solution $\{Y_n\}$ generated by the method converges in some sense to the theoretical solution $y(x)$ as the step length, h, approaches zero.

Definition (1.3.1): The linear multistep method (1.3.2) is said to be convergent for all y_n of the $\{y_n\}$ if and only if

$$\lim_{h\to 0} y_n = y(x_n), \text{ for all } x \in [a,b],$$

and for all solutions $\{y_n\}$ of the difference equation (1.3.2) satisfying starting conditions

$$y_\mu = A_\mu(h) \text{ for which } \lim_{h\to 0} A_\mu(h) = A,$$

$$\mu = 0,1,2 \ldots\ldots k-1.$$

1.3.5 Order and Error Constant

With linear multistep method (1.3.1), if we associate the linear difference operator L defined by

$$L[y(x),h] = \sum_{j=0}^{k} [\alpha_j y(x+jh) - h\,\beta_j y'(x+jh)], \quad ---(1.3.12)$$

where y(x) is an arbitrary function, continuously differentiable on [a,b]. Expanding the test function y(x+jh) and its derivative $y'(x + jh)$ as Taylor series about x, and collecting terms in (1.3.12) gives

$$L[y(x), h] = C_0 y(x) + C_1 h y'(x) + \ldots + C_q h^q y^{(q)}(x) + \ldots \quad ----- (1.3.13)$$

where the C_q are constants.

Definition (1.3.2): The difference operator (1.3.12) and the associated linear multistep method (1.3.2) are said to be of order P if, in (1.3.13), $C_0 = C_1 = \ldots = C_p = 0$, $C_{p+1} \neq 0$.

Since $C_{p+1} \neq 0$, it implies that C_{p+1} has an absolute significance. We call C_{p+1} the error constant.

1.3.6 Local And Global Truncation Error

Definition (1.3.3): The local truncation error at x_{n+k} of the method (1.3.2) is defined to be the expression $L[y(x_n); h]$ given by (1.3.12), when y(x) is the theoretical solution of the initial value problem (1.3.1). In other words, the truncation error is the quantity **T** which must be added to the true representation of the computed quantity in order that the result be exactly equal to the quantity we are seeking to generate.

That is, y(true representation) + **T** = y(exact).

In general we define the truncation error

$$T_{n+k} = C_{p+1} h^{p+1} y^{(p+1)} (x_n) + O(h^{p+2}) \quad \text{\_\_\_\_\_\_} (1.3.14)$$

where p is the order of the method.

The global truncation error involves all the truncation errors made at each application of the method, and depends in a complicated way on the coefficients of the method and on the initial value problem. It is this error which convergence demands shall tend to zero as $h \to 0$, $n \to \infty$, $nh = x_n = x_n - a$ remaining fixed.

1.3.6 Consistency and Zero - Stability

The linear multistep method (1.3.2) is said to be consistent if it has order $P \geq 1$.

We now introduce the first and second characteristic polynomials of the linear multistep method (1.3.2) defined as $\rho(r)$ and $\sigma(r)$ respectively, where

$$\left.\begin{aligned} \rho(r) &= \sum_{j=o}^{k} \alpha_j r^j, \\ \sigma(r) &= \sum_{j=o}^{k} \beta_j r^j \end{aligned}\right\} \quad \text{\_\_\_\_\_\_\_\_\_\_} (1.3.15)$$

Thus, a linear multistep method is consistent if and only if

$$\rho(1) = o, \quad \rho'(1) = \sigma(1).$$

If follows that for a consistent method, the first characteristic equation $\rho(r)$ always has a root at +1. And for a method to be zero-stable the root of the first characteristic polynomial $\rho(r)$ has modulus greater than one, and if every root with modulus one is simple. thus a linear multistep method is said to be convergent if it is consistent and zero-stable.

CHAPTER TWO

General Review of Numerical methods for Singular and Discountinuous Systems

2.1 Literature Review

The study of numerical treatment for singular and discountinuous initial value problem had been carried out by Lambert and Shaw[5]. They proposed that the theoretical solution to the initial value problem

$$y' = f(x,y),\ y(0) = 0$$

be represented by a perturbed polynomial of the form

$$F(x) = P_L(x) + \begin{cases} \rho|A + x|^N, & N \in \{0,1.....L\} \\ \text{Or} \\ \rho|A+x|^N, & N \in \{0,1.....L\} \end{cases}$$

They defined $P_L(x)$ as a polynomial of degree L and the second term on the right hand side as the perturbation term. A and N are the singularity parameters, with A controlling the location of the singularity and N determining the nature of the singularity.

Shaw[6] later extended or improved on the theoretical solution by a perturbed polynomial. He proposed the adoption of a multistep method, thereby eliminating the need to generate the higher derivatives analytically. In his improved method, singularity parameters can be obtained by solving a pair of non-liner equations.

Lambert and Shaw[7] provided an alternative procedure that was based on a local representatin of the theoretical solution to $y' = f(x,y)$ by a specialised form of rational function

$$F(x) = \frac{P_m(x)}{(b+x)},$$

where $P_m(x)$ is a polynomial of degree m. Thus, accordingly, the integration formulas which emanated from this rational function can cope with special singular initial value problem.

Luke et al [8] suggested in his study that the rational function thought of by Lambert and Shaw can be replaced by a generalized rational function

$$f(x) = \frac{P_\mu(x)}{Q_r(x)},$$

Here the singularities are specified by the zeros of $Q_r(x)$.

The theory of ordinary non-linear differential equations offers no clue as to the point or location and the nature of singularities in the solution of an equation. Gear and Osterby(9) proposed an efficient method based on a local error estimators to detect and locate a point of discountinuity without using the singularity function. They made a provisin to pass the discountinuity and restart the integration process.

Fatunla[10] discussed the numerical treatment for singular and discountinuous initial value problems by adopting the generalised rational function of Luke (1975). Fatunla suggested a rational function of a special kind and represented the theoretical solution y(x) locally by

$$F_k(x) = \frac{A}{1 + \sum_{j=1}^{k} a_j x^j}, \qquad k \geq 1,$$

where A, a_j are real coefficients. In this case the singularity can be obtained from the poles of $F_k(x)$. Hence, he developed a one-step method to approximate the solution of the initial value problem. Fatunla's one-step method reduces the problem of the solution of non linear equations at every integration step which is characterised by the Lambert and Shaw methods.

Fatunla [10] also suggested the use of non-polynomial methods in dealing with singular and discontinuous initial value problems. Here he adopted the specialised form of rational function of Lambert and Shaw [1968]. The specialized rational function of Lambert and Shaw was defined as

$$F(x) = \frac{P_m(x)}{(b + x)},$$

where $P_m(x)$ is a polynomial of degree m. Fatunla re-defined the above rational function as

$$F(x) = \frac{P_m(x)}{Q_v(x)},$$

where $P_m(x)$ and $Q_v(x)$ are polynomials of degree m and v respecitvely.

The polynomial $P_m(x)$ and $Q_v(x)$ are given as

$$P_m(x) = \sum_{r=0}^{m} a_r x^r$$

and

$$Q_v(x) = 1 + \sum_{r=1}^{v} b_r x^r$$

He specified the singularities by the zeros of $Q_v(x)$ and developed a two-step method to approximate the solution of the initial value problem with the error function $E_{mv}(x)$, given by

$$E_{mv}(x_{n+j}) = 0, \; j = 0,1....s+1.$$

Adeboye[11] studied a convergent one step method for initial value problems in which some components of the solution contain discontinuities based on the Obrechkoff's method. He adopted the Obrechkoff's general one-step method

$$Y_{n+1} = Y_n + \sum_{i=1}^{q} a_i h^i y^i_{n+1} + \sum_{i=1}^{p} b_i h^{(i)} y_n^{(i)}$$

and developed a one-step method by solving for a_i and b_i in the Obrechkoff's general one-step method. Adeboye's explicit on-step method is given by

$$Y_{n+1} = \frac{Y_n + hf_n}{1-h^2 f_n},$$

where h is the step length and $f_n = y'_n$. Even though, Adeboye did not specify the singularity function, the one-step method above is convergent and it is an improvement on Fatunla's predictor formula or a two-step integrator

$$Y_{n+2} = \frac{2y^2_{n+1} - 2y_n y_{n+1} + hy'_{n+1} y_n}{2y_{n+1} - 2y_n - hy'_{n+1}}$$

Fatunla and Aashikpelokhai[12] developed a one-step method which was based on rational approximation for initial value problems. The integrator does not involve the solution of linear equations. Fatunla [13] developed a fourth order integrator which is very effective at solving stiff and highly oscillatory initial value problems. However, integrator cannot cope well with singular initial value problems. Hence, Fatunla and Aashikpelokhai[12] thought of an integrator which can cope with singular problems as well as stiff problems and hence developed a fifth-order one-step method based on an operator U and defined by

$$[1 + q_1 x + q_2 x^2 + q_3 x^3) \; U(x) = P_0 + P_1 x + P_2 x^2$$

subject to the constraints

$$U[x_{n+j}] = Y_{n+j}, \; j = 0,1$$

They finally came up with the integrator

$$y_{n+1} = \frac{y_n + 60Uy^{(1)}{}_n h + [Ay^{(1)}{}_n + 30Uy^{(2)}{}_n]h^2 - Cy_n h^3}{60U + Ah + Bh^2 + Ch^3}.$$

2.2 Overview of Non-Polynomial Methods

The non-polynomial method was first suggested by Lambert and Shaw[5]. They proposed that the theoretical solution to the initial value problem of the form

$$y' = f(x,y), \qquad y_{(0)} = y_0 \quad \text{———} \quad (2.2.1)$$

be represented by either of the following perturbed polynomials

$$F(x) = P_m(x) + \begin{cases} \alpha |A+x|^N, & N \in (0,1.....m) \text{ or} \\ \alpha |A+x|^N \log|A+x|, & N \notin 0,1,..m \end{cases} \quad -(2.22)$$

with $P_m(x)$ a polynomial of degree m. They defined

$$P_m(x) = \sum_{j=0}^{m} a_j x^j \quad \text{————} \quad (2.2.3)$$

and the second term on the right hand side being the perturbation term. A and N are the singularity parameters, with A controlling the location of the singularity, while N determines the nature of the singularity.

Lambert and Shaw obtained a one-step methods of order (m+1) by imposing the constraints

$$F(x_{n+j}) = y(x_{n+j}), \; j = 0,1$$

$$F^{(s)}(x_n) = y^{(s)}(x_n), \; s = 0,1,....m+1$$

on the interpolating functions (2.2.2). Thus

$$y_{n+1} = Y_n + \sum_{j=1}^{m} \frac{h^j y^{(j)}{}_n}{j!} + \frac{(A+x_n)^{m+1} y_n^{(m+1)}}{\beta^N{}_m} \left[\left(1+\frac{h}{A+x_n}\right)^{N-1} - \sum_{j=1}^{m} \frac{\beta^N{}_{j-1}}{j!} \left(\frac{h}{A+x_n}\right)^j\right]$$

and

$$y_{n+1} = Y_n + \sum_{j=1}^{m} \frac{h^j}{j!} y^{(j)}{}_n (-1)^{M-N} \frac{(A+x_n)^{m+1} y_n^{(m+1)}}{N!(M-N)!} \; \mathbf{X}$$

$$\left[\left(1+\frac{h}{A+x_n}\right)^N \log\left(1+\frac{h}{A+x_n}\right) - \sum_{j=1}^{m}\left\{\frac{\beta^N_{j-1}}{j!}\left(\frac{h}{A+x_n}\right)^j \sum_{r=0}^{j-1}\frac{1}{N-r!}\right\}\right] \qquad \text{------ (2.2.4)}$$

where $\beta^m_j = m(m-1) \ldots\ldots (m-j),\ j > 0.$

They defined the local truncation error

$$t_{n+1} = \sum_{j=m+2}^{\infty}\left\{ y^{(j)}_n - \frac{\beta^{N-m-1}_{j-m-2}}{(A+x_n)^{j-m-1}}\, y_n^{(m+1)}\right\}\frac{h^j}{j!} \qquad \text{----(2.2.5)}$$

The singularity parameters can be obtained by the following:-

$$\left.\begin{aligned} N_{(n)} &= m+1+\frac{y_n^{(m+1)2}}{y_n^{(m+2)2} - y_n^{(m+1)}\,y_n^{(m+3)}} \\ &\text{and} \\ N_{(n)} &= -x_n+\frac{y_n^{(m+2)}}{y_n^{(m+2)2} - y_n^{(m+1)}\,y_n^{(m+3)}} \end{aligned}\right\} \qquad \text{---(2.2.6)}$$

Shaw[6] extended the discussion above to multistep methods, thereby eliminating the need to generate the higher derivative analytically. In this case, the singularity parameters can be obtained by solving a pair of non linear equations.

Luke et al [8] suggested the adoption of a generalized rational function :

$$F(x) = \frac{P_m(x)}{Q_n(x)},$$

He specified the singularities function by the zeros of $Q_n(x)$.

Fatunla[10] defined the polynomials $P_m(x)$ and $Q_n(x)$ as

$$P_m(x) = \sum_{r=0}^{m} a_r x^r \qquad (2.2.7a)$$

and $$Q_n(x) = 1 + \sum_{r=1}^{n} b_r a^r \qquad (2.2.7b)$$

He specified the error function $Em,n(x)$ as follows

$$Em,n(x) = Q_n(x)y(x) - P_m(x) \qquad (2.2.8)$$

On differentiating with respect to x, he obtained

$$E'm,n(x) = Q_n(x)y'(x) + Q_n'(x)y(x) - P'_m(x) \qquad (2.2.9)$$

He illustrated the development of integration algorithm with a case where m = n = 1 in (2.2.7) which gives

$$E_{11}(x)0 = (1 + b_1x)\ y(x) - (a_0 + a_1x) \qquad (2.2.10)$$

and $$E'_{11}(x) = (1+b_1x)\ y'(x) + b_1y(x) - a_1 \qquad (2.2.11)$$

Imposing the constraints

$$E_{11}(x_{n+j}) = 0,$$

That is, $E_{11}(x_{n+1}) = 0$

and $x_n = 0,\ x_{n+j} = j$

in (2..2.10) and (2.2.11) and replacing y'_j by hy'_j

$$
\left.
\begin{aligned}
Y_n &= a_0 && \text{(i)}\\
(1+b_1)y_{n+1} &= a_0 + a_1 && \text{(ii)}\\
(1+2b_1)y_{n+2} &= a_0 + 2a_1 && \text{(iii)}
\end{aligned}
\right\} 2.2.12
$$

$$(1+b_1)hy'_{n+1} + b_1y_{n+1} = a_1 \qquad \text{(iv)}$$

Substitute (i) and (iv) in (ii) gives

$$b_1 = \frac{y_{n+1} - y_o - hy'_{n+1}}{hy'_{n+1}} \qquad \text{-----------} \quad (2.2.13)$$

Adopting (ii) in (iii) gives

$$(1+2b_1)y_{n+2} = (1+b_1)y_{n+1} + a_1 \quad \_\_\_\_\_ (2.2.14)$$

Inserting (iv) and (2.2.13) in (2.2.14) he obtained what he called predictor formula

$$y_{n+2} = \frac{y^2_{n+1} - 2y_n y_{n+1} + hy'_{n+1} y_n}{2y_{n+1} - 2y_n - hy'_{n+1}} \quad \ldots\ldots\ldots\ldots \quad (2.2.15)$$

We shall adopt the above integration formula to perform some numerical experiments in chapter four of this work.

2.3 Overview of A Convergent Explicit One-step Method

Adeboye[11] developed a convergent explicit one-step method based on the Obrechkoff's one-step method. Obrechkoff developed an absolutely stable implicit one-step method of maximum order 2p, based on the first p derivatives of the Taylor's series expansion of y for the solution of initial value problem.

$$y' = \lambda y, \; y_{(0)} = y_0$$

He gives the interval of stability as $(-\infty, 0)$.

Adeboye[11] modified the Obrechkoff's method thus:

Obrechkoff's general one-step method is defined by

$$y_{n+1} = y_n + \sum_{i=1}^{q} a_i h^i y^{(i)}_{n+1} + \sum_{i=0}^{p} b_i h^i y^{(i)}_n \quad \text{(2.3.1)}$$

Hence

$$y_{n+1} = y_n + \sum_{i=1}^{2} a_i h^i y^{(i)}_{n+1} + \sum_{i=0}^{2} b_i h^i y^{(i)}_n \quad \text{(2.3.1)}$$

that is from (2.3.1), $q = 1,2,\ p = 0,1,2.$

From (2.3.2) he obtained

$$y_{n+1} = y_n + (a_1 + b_1)hy'_n + (a_1+a_2 + b_2)h^2y''_n \quad \text{(2.3.3)}$$

The Taylor's series expansion for y_{n+1} is given by

$$y_{n+1} = y_n + hy'_n + \frac{h^2}{2} y_n'' + \ldots$$

i.e. $$y_{n+1} = y_n + hy'_n + \frac{h^2}{2} y_n'' + \ldots \quad \text{(2.3.4)}$$

Equating the coefficients of equal powers of h in (2.3.3) and (2.3.4), we obtain

$$a_1 + b_1 = 1$$
$$a_1 + a_2 + b_2 = \tfrac{1}{2}$$

The above equations have four unknowns. He fixed one of the unknowns arbitrarily to reduce the equation to a one-parameter family of solutions. Hence, in putting $b_2 = 0$, then

$$a_1 = 1 - b_1$$
$$a_2 = \tfrac{1}{2} - a_1 = \tfrac{1}{2} - 1 + b_1 = b_1 - \tfrac{1}{2}.$$

Substituting in (2.3.3), we obtained

$$y_{n+1} = y_n + (1-b)y'_{n+1} + h^2(b - ½)y_{n+1}'' + hb_1y'_n \quad \text{--2.3.5)}$$

Equation (2.3.5) is a one-parameter family of second order methods.

Adeboye[11] illustrates the development of an explicit one-step scheme for initial value problems by considering the initial value problems

$$y' = y^2, \; y(_0) = 1 \quad \_\_\_\_\_\_ \; (2.3.6)$$

and $$y' = 1 + y^2, \; y(_0) = 1 \quad \_\_\_\_\_\_ \; (2.3.7)$$

In the solutions of (2.3.6) and (2.3.7) there are discontinuities at $x = 1$ and $x = \pi/4$ respectively. He adopted the method (2.3.5) by differentiating (2.3.6) and (2.3.7) to obtain

$$y'' = 2y' \quad \_\_\_\_\_\_\_ \; (2.3.8)$$

Substituting for (2.3.5), y_{n+1} "its equivalence of y") in (2.3.8), we obtain

$$y_{n+1} = y_n + (1-b_1)y'_{n+1} + 2(b_1 - ½)y_{n+1}y'_{n+1} + hb_1y'_n$$

Expanding y_{n+1} in powers of h about x_0, and using only the first term of the expansion gives

$$y_{n+1} = y_n + (1-b_1)y'_n + 2h^2(b_1 - ½)y_{n+1}y'_{n+1} + hb_1y'_n$$

He further put $b_1 = 1$ to obtain

$$y_{n+1} = y_n + h^2 \, y'_{n+1} \, y_{n+1}hy'_n$$

$$y_{n+1} = (1-h^2 \, y'_{n+1}) = y_nhy'_n$$

$$y_{n+1} = \frac{y_n + hy'_n}{1-h^2\,y'_{n+1}} \quad \text{or} \quad y_{n+1} = \frac{y_n + hf_n}{1-h^2 fn} \quad \ldots (2.3.9)$$

The method (2.3.9) is a second order one-step scheme for initial value problems of class one. The scheme is convergent. We shall illustrate the adoption of the above scheme to some initial value problems in chapter four of this write up.

2.4 Overview of Inverse Polynomial Methods

Even though the scheme based on rational approximations are quite effective for the solution of singular initial value problems, the derivation of these schemes are very tedious and complicated. In view of this, Fatunla[10] suggested the use of inverse rational function. He approximated theoretically the solution y(x) to the initial value problem

$$y' = f(x,y),\; y_{(0)} = y_0$$

locally by

$$F_k(x) = \frac{A}{1 + \sum_{j=1}^{k} a_j x^j}, \quad k \geqslant 1 \quad \text{\_\_\_\_\_\_} \quad (2.4.1)$$

where A, a_j are real coefficients to be determined.

He defined the error function $E_k(x)$ as

$$E_k(x) = (1 + \sum_{j=1}^{k} a_j x^j)y(x) - A \quad \text{\_\_\_\_\_\_} \quad (2.4.2)$$

which on differentiation gives

$$E'_k(x) = (1 + \sum_{j=1}^{k} a_j x^j)y'(x) + (\sum_{j=1}^{k} j a_j x^{j-1})y(x) \quad \text{\_\_\_\_\_\_} (2.4.3)$$

The imposition of the constraints

$$E_k(x_{n+i}) = 0, \; i = 0,1 \ldots\ldots k$$

and the transformation

$x = x_0 + th$, gives the integration formula

$$y_{n+k} = \frac{y_n}{1 + \sum_{j=1}^{k} k^j a_j}, \quad \text{\_\_\_\_\_\_} (2.4.4)$$

He obtained the numerical values of the components of the k-vector $a = (a, a_2 \ldots a_k)^T$, by ensuring that the interpolating function (2.4.1) satisfies the differential equation at k points

$\{x_{n+j}, j = 0, 1 \ldots\ldots k - 1\}$. This implies

$$E'(x_{n+j}) = 0, \; i = 0, 1 \ldots\ldots k - 1 \quad \text{\_\_\_\_\_\_} (2.4.5)$$

He adopted the transformation $x = x_0 + th$ in (2.4.5) and replaced y'_i by hy'_i to obtain linear system of k dimension:

$$Ra = b \quad \text{\_\_\_\_\_\_} (2.4.6)$$

where R is a k by k matrix with its elements specified as

$$R_{ij} = hy'_1 i^j + j i^{j-1} y_i, \; i = 0,1 \ldots k-1 \quad \text{\_\_\_\_\_\_} (2.4.7)$$

and b is a k-vector whose ith element is

$$b_i = -hy'_i, \quad i = 0,1 \ldots k-1 \quad \text{\_\_\_\_\_\_} (2.4.8)$$

The system (2.4.6) has unique solution if

$$\det(R) \neq 0.$$

If the det(R) = 0, then there is a strong indication of a singularity. The singularity can be obtained from the poles of $F_k(x)$.

Fatunla developed a one-step method by setting k = 1 in system (2.4.4). that is,

$$y_{n+1} = \frac{y_n}{(1 + a_i)}, \quad \text{——— (2.4.9)}$$

Using (2.4.6), he obtained

$$R_{01}a_1 = b_0 \quad \text{——— (i)}$$

From (2.4.7),

$$R_{01} = y_0 \quad \text{———(ii)}$$

and from (2.4.8),

$$b_0 = -hy'_0 \quad \text{———(iii)}$$

Substituting (ii) and (iii) into (i) gives

$$a_1 = -hy'_0/y_0$$

Substituting for (a_1) in (2.4.9) gives

$$y_{n+1} = \frac{y_n^2}{y_n - hy'_n},$$

He specified the local truncation error by

$$t_{n+1} = \frac{(\tfrac{1}{2}y_n y'_n - y^2_n)}{y_n - hy'_n} h^2, \quad |y(x)| + |y'(x)| \neq 0$$

This suggests that (2.4.10) is at least of order $P \geq 1$, provided $|y_n| \neq 0$. In a situation where y_n vanishes the meshzise h, can be adjusted. We shall perform numerical experiment using the integrator (2.4.10) in chapter four.

2.5 Overview of A fifth Order L-Stable Numerical Methods

Fatunla and Aashikpelokhai[12] developed a one-step method for first order initial value problems. The integrator does not involve the solution of linear equations. Fatunla [13] developed a highly accurate fourth order explicit one-step numerical scheme which is L-stable. The method is given by

$$y_{n+1} = y_n + Rf_n + Sf_n^{(1)} \qquad \text{———} \quad (2.5.1)$$

where the matrices R and S are defined as

$$R = a_2\phi - a_1\psi$$

$$S = \phi + \psi$$

and the diagonal matrices ϕ , ψ have entries given by

$$\phi_i = \frac{e^{a_{1i}h} - 1}{a_{2i}[a_{1i} + a_{2i}]} \qquad i = 1, (1)m$$

$$\psi_i = \frac{e^{-a_{2i}h} - 1}{a_{2i}[a_{1i} + a_{2i}]}, \qquad i = 1, (1)m$$

The stiffness/oscillatory parameters a_{1i} and a_{2i} are evaluated using

$$\begin{bmatrix} f_{ni}^{(2)} & f_{ni}^{(1)} \\ f_{ni}^{(1)} & f_{ni} \end{bmatrix} \begin{bmatrix} a_{2i} & -a_{1i} \\ a_{2i} & -a_{1i} \end{bmatrix} = \begin{bmatrix} -f_{ni}^{(3)} \\ -f_{ni}^{(2)} \end{bmatrix}$$

The integrator (2.5.10) is very effective at solving stiff and highly oscillatory initial value problems. Hence Fatunla and Aashikpelokhai[12] thought of an integrator which can cope well with singular problems as well as stiff problems. They developed the integrator by considering the operator U defined by

$$(1+ q_1x + q_2x^2 + q_3x^3)U(x) = P_0 + P_1x + P_2x^2 \quad \ldots(2.5.2)$$

subject to the constraints

$$U(X_{n+j}) = y_{n+j},\ j = 0,1 \text{ --------}(2.5.3)$$

They further inposed the condition

$$y_n = y(x_n) \text{--------------}(2.5.4)$$

The integrator is a one - step method. Therefore it is expected to use the value y_n to compute y_{n+1} as an approxination to $y(x_{n+1})$. To achieve this, they determined the relationship between y_n and y_{n+1} using Taylor series expansion of $y(X_{n+1})$ and y_{n+1} about $X = X_n$ with

$$h_n = X_{n+1} - X_n \quad \ldots\ldots\ldots\ldots\ldots(2.5.5)$$

To evaluate (q_1, q_2,q_3 P_0, P_1,P_2) and for y_{n+1} to be good approxination to $y(X_{n+1})$, they impose the constraints that the power series of

$$y_{n+1} = [\sum_{\alpha=0}^{2} p_\alpha h^\alpha (n+1)^\alpha] [\sum_{i=0}^{\infty} (-1)^i \{1 + \sum_{\beta=1}^{3} q_\beta h^\beta (n+1)^\beta\}^i] \quad (2.5.6)$$

and

$$y(X_{n+1}) = \sum_{r=0}^{\infty} \frac{h^r y^r (x)}{r!} \quad \text{------}(2.5.7)$$

, where $x_n = nh$,

$$y^{(r)}(X_n) = \frac{d^r y(x)}{dx^r}\Big|_{x=X_n}$$

must concide for h^r, $r=0,1\ldots5$.

This demand makes the integrator to be, of order at least five. Equating the terms of the Taylor series given by (2.5.6) and (2.5.7) gives

$$P_0 = y_n \quad \text{---------}(2.5.8)$$

$$P_1 x_{n+1} = h y_{n(1)} + q_1 y_n x_{n+1} \quad \text{----}(2.5.9)$$

$$P_2 x^2_{n+1} = \frac{h^2 y_n^{(2)}}{2!} + h y_n^{(1)} q_1 x_{n+1} + y_n q_2 x^2_{n+1} \text{--}(2.5.10)$$

$$q_1 x_{n+1} = \frac{(a_1+a_2+a_3)h}{60(u_1+u_2+u_3)} \quad \text{----------}(2.5.11)$$

$$q_2 x^2_{n+1} = \frac{(b_1+b_2+b_3)h^2}{60(u_1+u_2+u_3)} \quad \text{-----------}(2.5.12)$$

$$q_3 x^3_{n+1} = \frac{(C_1+C_2+C_3)h^3}{60(u_1+u_2+u_3)} \quad \text{------------}(2.5.13)$$

where the a_i, b_i, c_i and u_i are given by

$$\left.\begin{aligned} a_1 &= 36\ y_n^{(5)}\ [2y_n^{(1)2} - y_n^{(2)} y_n] \\ a_2 &= 60\ y_n^{(3)}\ [y_n^{(4)} y - 4^{(3)} y_n^{(1)}] \\ a_3 &= 180\ y_n^{(2)} y(3) y_n^{(2)} - y_n^{(4)} y_n^{(1)}] \end{aligned}\right\} \text{-----}\ (2.5.14)$$

$$b_1 = 15\ y_n^{(4)}[4y_n^{(3)2}\ y_n^{(1)} - y_n^{(4)}y_n]$$
$$b_2 = 12\ y_n^{(5)}\ [y_n^{(3)}y_n - 3y^{n(2)}y_n^{(1)}] \quad \Big\}----(2.5.15)$$
$$b_3 = 30\ y_n^{(2)}[3y_n^{(4)}y_n^{(2)} - 4y_n^{(3)2}]$$

$$c_1 = 15\ y_n^{(4)}\ [y_n^{(1)}y_n^{(4)} - 2y_n^{(2)}y_n^{(3)}]$$
$$c_2 = 10\ y_n^{(5)}\ [4y_n^{(3)2}y_n - 3y_n^{(2)}y_n^{(5)}] \quad \Big\}----(2.5.16)$$
$$c_3 = 3\ y_n^{(5)}[6y_n^{(2)2} - 4y_n^{(3)}\ y_n^{(1)}]$$

$$u_1 = 3\ y_n^{(4)}\ [y_n^{(2)}y_n - -2y_n^{(1)2}]$$
$$u_2 = 4\ y_n^{(3)})\ [3y_n^{(2)}y_n^{(1)} - y_n^{(3)}y_n] \quad \Big\}-----(2.5.17)$$
$$u_3 = 3\ y_n^{(2)}[4y_n^{(3)}y^{(1)}{}_n - 6y_n^{(2)2}]$$

Adopting these results in (2.5.2) and (2.5.3) they obtained the integrator,

$$y_{n+1} - y_n = \frac{60Uy_n^{(1)}h + [Ay_n^{(1)} + 30Uy_n^{(2)}]h^2 - Cy_nh^3}{60U + Ah + Bh^2 + Ch^3} \quad --(2.5.18)$$

where

$$A = \sum_{i=1}^{3} a_i$$

$$B = \sum_{i=1}^{3} b_i$$

$$C = \sum_{i=1}^{3} c_i \qquad \Big\}\ ---(2.5.19)$$

$$U = \sum_{i=1}^{3} u_i$$

and the a_i, b_i, c_i and u_i are as given respectively by (2.5.14 -2.5.17).

The integrator (2.5.18) is convergent and L-stable.

CHAPTER THREE

3.0 DEVOLOPMNET OF A NEW NUMERICAL INTEGRATION FOR SINGULAR AND DISCONTINOUS SYSTEMS

3.1 INTRODUCTION

Fatunla [10] suggested the adoption of a rational function

$$F(x) = \frac{P_m(x)}{Q_n(x)}, \text{ where}$$

$$P_m(x) = \sum_{r=0}^{m} a_r x^r \text{ and } Q_n(x) = 1 + \sum_{r=0}^{n} b_r x^r$$

He approximated the theoretical solution y(x) to the initial value problem

$$y' = F(x,y), \; y(0) = y_0 \text{ ----------- } (3.1.1)$$

locally by

$$F_k(x) = \frac{A}{1 + \sum_{j=1}^{k} a_j x^j}, \quad K \geq 1, \text{ ----------} (3.1.2)$$

where A, a_j are real constants.

Fatunla's interpolating function (3.1.2 is modified thus:

We can also approximate the theoretical solution y(x) locally by

$$F_k(x) = \frac{A}{1 + \sum_{j=0}^{k-1} a_j x^j}, \quad K > 1, \text{ -------------- } (3.1.3)$$

where A, aj are real coefficients. That is

$$y(x) = F_k(x)$$

From equation (3.1.3) we define the error equation as

$$E_k(x) = (1 + \sum_{j=0}^{k-1} a_j x^j) y(x) - A \quad \text{--------(3.1.4)}$$

If we differentiate (3.1.4) with respect to x, we have

$$E'_k(x) = (1 + \sum_{j=0}^{k-1} a_j x^j) y'(x) + (j \sum_{j=0}^{k-1} a_j x^{j-1}) y(x) \quad \text{---- (3.1.5)}$$

We now impose the following constraint

$$E_k(x_{n+i}) = 0, \ i = 0, 1\text{----} \ k-1$$

and also adopt the transformation

$x_n = 0$, $x_{n+j} = j$ in equation (3.1.4) in order to obtain the value of A in the numerator of (3.1.3)

That is

$$(1 + \sum_{j=0}^{k-1} a_j x^j) y(x) - A = E_k(x)$$

$$\Rightarrow (1 + \sum_{j=0}^{k-1} a_j (0)) y(0) - A = 0$$

$$y(0) + y(0) \sum_{j=0}^{k-1} a_j (0) - A = 0$$

$$y(0) - A \doteq 0$$

$$y(0) = A$$

Therefore $A \cong y_n$

With $A \cong Y_n$, then (3.1.3) becomes

$$F_k(x) = \frac{Y_n}{1 + \sum_{j=0}^{k-1} a_j x^j} \quad \text{-----------}(3.1.6)$$

In order to obtain a k - step non linear multi- step formula, we simply replace x by k in (3.1.6. Thus,

$$y_{n+k} = \frac{Y_n}{1 + \sum_{j=0}^{k-1} a_j k^j}, \quad K > 1 \quad \text{----------}(3.1.7)$$

It now remains to find the numerical values of the components of the k - vector $a = (a_1, a_2, a_3 \ldots a_{k-1})^T$. We can achieve this by ensuring that the interpolating function (3.1.3) satisfies the differential equation at K points $\{x_{n+i}, i = 0\ 1, 2, \ldots k-1\}$.

This implies,

$$E'(x_{n+i}) = 0, \quad i = 0\ 1, \ldots.\ k-1 \quad \text{--------}\ (3.1.8)$$

If we adopt the transformation, $x_n = 0$, $x_{n+i} = i$ in equation (3.1.8) and replacing y_i' by hy_i' we obtain the following linear system in k dimension.

$Ra = b$ ....(3.1.9),

where R is a k by k matrix, and b is a k-vector. The elements of matrix R and vector b are specified as follows using (3.1.5) and the transformation above.

That is ,

$$\left(1+\sum_{j=0}^{k-1} a_j x^j\right) y'(x) + \left(j\sum_{j=0}^{k-1} a_j x^{j-1}\right) y(x) = E'_k(x)$$

$$\text{Then } y'(x) + \left(\sum_{j=0}^{k-1} a_j x^j\right) y'(x) + \left(j\sum_{j=0}^{k-1} a_j x^{j-1}\right) y(x) = 0$$

$$hy_i' + h_i^j y_i' + j_i j-1 \, y_i = 0$$

$$h_i^j y_i' + j_i j-1 \, y_i = hy_i'$$

$$R_{ij} = h_i^j y_i' + j_i j-1 \, y_i, \quad \left.\begin{array}{l} i = 0,1\ldots k-1 \\ j = 0, 1\ldots k-1 \end{array}\right\} \ldots (3.1.10)$$

and $b_i = -hy_i'$, $i = 0, 1\ldots\ldots k-1$ ....(3.1.11)

The system (3.1.9) has a unique solution

if $\det.(R) \neq 0$ ------------ (3.1.12)

In a situation where $\det(R) = 0$, there is a strong indication of the existence of singularity, and we can over step this singularity by adjusting the step-size.

The singularity can be obtained from the poles of $F_k(x)$

3.2 THE PROPOSED NUMERICAL INTEGRATOR

The proposed integrator shall be a two-step numerical integrator. That is by setting k = 2 in (3.1.7). we have

$$y_{n+2} = \frac{Y_n}{1 + \sum_{j=0}^{1} 2^j a_j}$$

$$y_{n+2} = \frac{Y_n}{1 + a_0 + 2a_1} \quad \text{-----------(3.2.1)}$$

We shall now find the value of a_0 and a_1 using equations (3.1.10) and (3.1.11)

That is, $R_{00}\ a_0 = b_0$ --------(3.2.2)

But $R_{00} = 0$ and $b_0 = -\ h\ y_0'$

Since $R_{00} = 0$, there is no unique solution to (3.2.2) by (3.1.12) above. Hence there is an indication of existance of singularity. To overstep this we go further to find the value of a_1 and consider a_0 to be zero.

That is $R_{11}\ a_1 = b_1$ -------(3.2.3)

$R_{11} = hy'_1 + y_1$

$b_1 = hy'_1$

$\therefore\ (hy'_1 + y_1)a_1 = -hy'_1$

$$a_1 = \frac{-hy'_1}{hy'_1 + y_1} \qquad \text{-----------(3.2.4)}$$

Inserting (3.2.3) into (3.2.1), we have

$$y_{n+2} = \frac{y_n}{1 - \dfrac{2hy'}{hy'_1 + y_1}} = \frac{y_n}{\dfrac{hy'_1 + y_1 - 2hy'_1}{hy'_1 + y_1}}$$

$$\therefore\ y_{n+2} = \frac{y_n(hy'_1 + y_1)}{y_1 - hy'_1} \qquad \text{------(3.2.5)}$$

$$y_{n+2} \cong \frac{y_n(hy'_{n+1} + y_{n+1})}{y_{n+1} - hy'_{n+1}}$$

$$\therefore\quad y_{n+2} \cong \frac{y_n(hf_{n+1} + y_{n+1})}{y_{n+1} - hf_{n+1}} \qquad \text{------(3.2.6)}$$

(3.2.6) is the proposed two-step numerical integrator.

3.3 CONVERGENCE OF THE METHOD

Theorem: A two-step numerical integrator of the form

$$y_{n+2} = \frac{y_n(hf_{n+1} + y_{n+1})}{y_{n+1} - hf_{n+1}} \qquad \text{------(3.3.1)}$$

is convergent if and only if :

i. *it is consistent*

ii. *it is zero stable*

PROOF

We shall establish the convergence of the method by showing that the method is consistent and zero - stable.

i. The integrator (3.3.1) can be written as

$$y_{n+2} = \frac{y_n(hf_{n+1} + y_{n+1})}{y_{n+1} - hf_{n+1}}$$

$$y_{n+2}(y_{n+1} - hf_{n+1}) = y_n(hf_{n+1} + y_{n+1})$$

$$y_{n+2}\, y_{n+1} - hy_{n+2}\, f_{n+1} = hy_n f_{n+1} + y_n y_{n+1}$$

$$y_{n+2}\, y_{n+1} - y_n y_{n+1} = hy_n f_{n+1} + hy_{n+2} f_{n+1}$$

$$y_{n+1}(y_{n+2} - y_n) = hf_{n+1}(y_n + y_{n+2})$$

So that $$\frac{y_{n+1}(y_{n+2} - y_n)}{y_n + y_{n+2}} = hf_{n+1} \qquad \text{------(3.3.2)}$$

We now consider the first and second characteristics equations $\rho(r)$ and $\sigma(r)$ of (3.3.2)

That is,

$$\rho(r) = \frac{r(r^2 - r^0)}{r^2 + r^0} = \frac{r^3 - r}{r^2 + 1}$$

$$\therefore \quad \rho(r) = \frac{1 - 1}{1 + 1} = 0$$

And $\rho'(r) = \dfrac{(r^2+1)(3r^2-1)-(r^3-r)(2r)}{(r^2+1)^2}$

$\rho'(1) = \dfrac{(1+1)(3-1)-(1-1)(2)}{(1+1)^2} = \dfrac{2x2-0}{4} = 1$

Now, $\sigma(r) = r$

This implies that $\sigma(1) = 1$

Hence $\rho'(1) - \sigma(1) = 1-1 = 0$

Since,

$\rho'(1) = 0$ and $\rho'(1) - \sigma(r) = 0$,

it implies that the integrator is consistent.

ii. From the first characteristics equation of (3.3.2)

$$\rho(r) = \frac{r(r^2-1)}{r^2+1} = 0$$

It implies that $r(r^2-1) = 0$.

Hence $r = 0$ or $r = r \pm 1$

Since the first characteristics equation of $\rho(r)$ has root with modulus less than one and the roots with modulus one each are simple roots, then the integrator is zero - stable.

Therefore the two step numerical integrator is convergent since it is shown to be consistent and zero-stable.

CHAPTER FOUR

4.0 NUMERICAL SOLUTIONS FOR SINGULAR AND DISCONTINUOUS SYSTEMS.

4.1 SPECIFIC NUMERICAL EXAMPLES OF SINGULAR AND DISCONTINUOUS SYSTEMENS USING THE NEW SCHEME

Here we shall solve some initial value problems in which some compnents of the solution contain.discontnuities.

Problem I. Solve $y' = 1 + y^2$, $y(0) = 1$

Solution

The exact solution is $y = \tan\left(x + \frac{\pi}{4}\right)$

we use $h = 0.05$ and generate y_1 from the exact solution.

That is, $y_1 = \tan\left(0.05 + \frac{\pi}{4}\right) = 1.10535559$

From the integrator

$$y_{n+2} = \frac{(hf_{n+1} + y_{n+1})}{y_{n+1} - hf_{n+1}}$$

Thus, for example by putting $y_1 = 1.10535559$, we obtain:

$$y_2 = \frac{y_0(hf_1 + y_1)}{y_1 - hf_1} = \frac{1.216446139}{0.9942650412} = 1.223462647$$

$$y_3 = \frac{y_1(hf_2 + y_2)}{y_2 - hf_2} = \frac{1.490357231}{1.098619605} = 1.356572579$$

Table 4.1 shows the performance of the integrator against the theoritical solution.

TABLE 4.1

X	EXACT SOLUTION	NEW SCHEME
0.05	1.10535559	1.10535559
0.10	1.223048888	1.223462647
0.15	1.356087851	1.356572579
0.20	1.508497647	1.509573919
0.25	1.685796417	1.687119434
0.30	1.8957655123	1.898012479
0.35	2.2.14974764	2.152670853
0.40	2.464962757	2.469554488
0.45	2.868884028	2.875314481
0.50	3.408223442	3.418434019
0.55	4.169364046	4.1854220
0.60	5.331855223	5.360482452
0.65	7.3404436575	7.398142675
0.70	11.6813738	11.83889669
0.75	28.23825285	29.24158055
0.80	-68.47966835	-62.8918434
0.85	-15.45789164	-15.13357206
0.90	-8.687629547	-8.576871132
0.95	-6.020299716	-5.96331911
1.00	-4.588037825	-4.552159575

There is a simple pole (singularity) at the point $x = \frac{\pi}{4}$.

Problem II Solve $y' = y^2$, $y(0) = 1$

Solution

The exact solution is $y = \frac{1}{1-x}$.

We use unique meshsize h = 0.1 and generate y_1.

That is , $y_1 = \frac{1}{1-0.1} = 1.11111111$.

There is discontnuity at the point x = 1

With $y_1 = 1.11111111$ we obtain

$$y_2 = \frac{y_0(hf_1+y_1)}{y_1 - hf_1} = \frac{1.234567901}{0.987654321} = 1.250000$$

Thus, table 4.2 shows the performance of the integrator against the theoritical solution.

Table 4.2

X	EXACT SOLUTION	NEW SCHEME
0	1	1
0.1	1.11111111	1.11111111
0.2	1.250000	1.240000
0.3	1.428571428	1.428571428
0.4	1.66666667	1.66666667
0.5	2.000000	2.000000
0.6	2.500000	2.500000
0.7	3.333333	3.3333333
0.8	5.000000	5.000000
0.9	10.000000	10.000000
1.0	∞	∞

PROBLEM III Solve $y' = xy^2$, $y(0) = 2$

Solution

The theoritical solution to this proble is $y = \frac{2}{1-x^2}$. It has simple poles (singularities) at the point $x = \pm 1$. The meshsize for this problem is $h = 0.1$. By generating

$$y_1 = \frac{2}{1-(0.1)^2} = 2.02020202,$$

then we obtain by the integrator $y_2 = 2.082474227$

Table 4.3 shows the performance of the integrator aganist the theoritical solution

Table 4.3

X	EXACT SOLUTION	NEW SCHEME
0	2.00000	2.000000
0.1	2.02020202	2.02020202
0.2	2.08333333	2.0824744227
0.3	2.197802198	2.195796171
0.4	2.380952381	2.376183322
0.5	2.66666667	2.657045863
0.6	3.1250600	3.106887568
0.7	5.921568627	3.874638377
0.8	5.5555556	5.41943779
0.9	10.52631579	9.80597169
1.0	$+\infty$	86.55115567
1.1	-9.523809524	-12.35782902
1.2	-4.545454545	-9.663164322

4.2 Comparison of the results with some established Schemes

For the initial value problem

$y' = 1+y^2,\ y(0) = 1,$

the performance of the integrator is compared with Fatunla [10], Adeboye [II] and Fatunla and Aashikpoelokhai [12] in table 4.4 below.

Table 4.4

X	EXACT SOLUTION	NEW SCHEME	FATUNLA[10]	ADEBOYE[11]	FATUNLA & AASHIKPELOKAI [12]
0.10	1.22304888	1.223462647	1.23530451	1.223433967	1.22304888
0.20	1.508497647	1.509573919	1.537684973	1.5099500011	1.50849765
0.30	1.8957655123	1.898012479	1.951571978	1.89853126	1.89576512
0.40	2.464962757	2.469554488	2.56946039	2.469199634	2.46496276
0.50	3.408223442	3.418434019	3.621678307	3.417521518	3.40822344
0.60	5.331855223	5.360482452	5.888280275	5.35733987	5.33185522
0.65	7.3404436575	7.398142675	8.446889	7.39121204	7.34043658
0.70	11.83889669	11.83889669	14.774102	11.81602726	11.6813738
0.75	28.23825285	29.24158055	57.272939	29.064451	28.2382529
0.80	68.47966835	-62.8918434	-30.7186028	-64.0294308	-68.4796683
0.90	-8.6876295	-8.575971	-7.521752	-8.581515	-8.6876295
1.00	-4.588037	-4.552159	-4.244590	-4.550432	-4.588037

The table above verifies that Fatunla and Aashikpelokai [12] has better performance than the new scheme, FAtunla [10] and Adeboye [11].

We now compare the performance of the integrator with Adeboye [11] and Fatunla [10] for the solution of the initial value problem $y' = y^2$, $y(0) = 1$ in table 4.5

TABLE 4.5

X	**EXACT SLOLUTION**	**NEW SCHEME**	**ADEBOYE [11]**	**FATUNLA [10]**
0	1.000000	1.00000	1.000000	1.0000000
0.1	1.11111111	1.11111111	1.11111111	1.111111111
0.2	1.250000	1.2499988	1.24993925	1.24993925
0.3	1.428571428	1.428571428	1.428571428	1.373632654
0.4	1.6666667	1.6666667	1.666665	1.592365127
0.5	2.00000	2.0000000	1.9999998	1.893951333
0.6	2.50000	2.5000000	2.500000	2.336466749
0.7	3.333333	3.3333333	3.333333	3.048811424
0.8	5.000000	5.0000000	4.9999998	4.386028938
0.9	10.000000	10.0000000	10.0000000	7.812703145
1.0	∞	∞	∞	35.71853141

Table 4.5 shows that both the integrator and Adeboye [11] performed better for the above initial value problem. The local truncation error is zero in each step. This implies that the two schemes are better. Fatunla[10] performance compared with theoretical solution indicates that the scheme performs well at the first few steps. There are some significant global errors before the point of discontnuity.

In table 4.6 we compare the performance of the integrator with Adeboye[11] and Fatunla[10] for the initial value problem:

$y' = y^2$, $y(0) = 2$

TABLE 4.6

X	EXACT SLOLUTION	NEW SCHEME	ADEBOYE[11]	FATUNLA [10]
0	2.000000	2.00000	2.000000	2.0000000
0.1	2.02020202	2.02020202	2.000000	2.000000
0.2	2.08333330	2.08247420	2.0481927	2.0408163
0.3	2.19780222	2.19579620	2.1501350	2.1276596
0.4	2.3809523	2.3761833	2.3210178	2.272772
0.5	2.666667	2.6570458	2.5923643	2.500000
0.6	3.1250000	3.1068876	3.0302021	2.8571429
0.7	3.1250000	3.8746384	3.789992701	3.4482759
0.8	5.5555556	5.4194374	5.3314222	4.5454545
0.9	10.5263158	9.8059072	9.8437399	7.14285715
1.0	∞	86.5511557	145.1418592	20.00002
1.1	-9.5238095	-12.35782902	-10.73996318	-19.99998
1.2	-4.5454544	-9.6631643	-7.24731337	-6.2499998

Table 4.6 shows the high performance of the integrator and Adeboye [11] over that of Fatunla [10] at the uniform meshsize h = 0.1. Fatunla [10] gives rise to results which are still less accurate than the integrator and Adeboye[11].

4.3 ERRORS IN COMPUTATIONAL RESULTS

The local truncation errors existing in the computation of problem I is shown in table 4.7 below. The local truncation error is computed by

Error = | y(x,h) - y(x) |, where y(x) is the theoritcal solution and y(x,h) is the numerical solution by the scheme.

TABLE 4.7

X	EXACT SOLUTION	ERROR IN INTEGRATOR	ERROR IN FATUNLA[10]	ERROR IN ADEBOYE[11]	ERROR IN FATUNLA & AASHIKPEKAI [12]
0.10	1.22304888	4.137(-4)	1.228(-2)	3.857(-4)	2.0 (-10)
0.20	1.508497859	1.076(-3)	2.918(-1)	1.002(-3)	2.0 (-10)
0.30	8.895765123	2.247(-3)	5.580(-2)	2.087(-3)	2.0 (-10)
0.40	2.46962757	4.592(-3)	1.045(-1)	4.237(-3)	2.0(-10)
0.50	3.40822344	1.021(-2)	2.135(-1)	9.321(-3)	3.0(-10)
0.60	5 .331855223	2.863(-2)	5.564(-1)	2.604(-2)	5.0(-10)
0.65	7.34046575	5.771(-2)	1.107(0)	5.072(-2)	7.0(10)
0.70	11.6813738	1.003(0)	3.092(0)	1.349(-1)	1.0(-9)
0.75	28.23825285	5.587(0)	2.903(1)	8.276(-1)	4.0(-9)
0.80	-68.4796683	3.243(-1)	3.776(1)	4.053(-1)	2.0(-10)
0.90	-8.68766295	1.107(-1)	1.666(0)	1.062(-1)	2.0(-10)
1.0	-4.588037	3.587(-2)	3.421(-1)	7.643(-3)	2.0(-10)

Index a(-b) = a $x10^6$

From the table we notice that Fatunla and Aashikpelokai[12] results show exceedingly high performance. The global errors are highly negligible. We also observe that the table shows that smaller meshsize h produce small global errors at each mesh point.

Table 4.8 shows the computational errors in the integrator, Adeboye[11] and Fatunla[10] for problem II above.

Problem II: $y' = y^2$, $y(0) = 1$

TABLE 4.8

x	EXACT SOLUTION	ERROR IN INTEGRATOR	ERROR IN ADEBOYE[11]	ERROR IN FATUNLA[10]
0	1.0	0	0	0
0.1	1.111111111	0	0	0
0.2	1.25000	0	0	6.075(-5)
0.3	1.428571428	0	0	5.492(-2)
0.4	1.6666667	0	0	7.430(-2)
0.5	2.000	0	0	1.060(-1)
0.6	2.5000	0	0	1.635(-1)
0.7	3.3333	0	0	2.845(-1)
0.8	5.0000	0	0	6.1409(-1)
0.9	10.000	0	0	2.187(0)
1.0	∞	0	0	-

We observe from the table above the exceedingly high accuracy in the results of the integrator and Adeboye[11]. We also notice that smaller meshsize h produce smaller global errors.

We compute the computational errors in the result of problem III as it is shown in table 4.9 below.

Problem III $y' = xy^2$, $y(0) = 2$.

TABLE 4.9

X	EXACT SOLUTION	ERROR IN INTEGRATOR	ERROR IN ADEBOYE[11]	ERROR IN FATUNLA[10]
0	2.0	0	0	0
0.1	2.02020202	0	-2.02(-1)	-2.02(-1)
0.2	2.08333333	-8.591(-4)	-3.514(-2)	-4.25(-2)
0.3	2.197802	-2.2261(-3)	-4.788(-2)	-7.036(-2)
0.4	2.3809523	-4.769(-3)	-5.993(-2)	-1.082(-1)
0.5	2.666667	-9.621(-3)	-7.43(-1)	-1.666(-1)
0.6	3.125000	-1.811(-2)	-9.479(-2)	-2.678(-1)
0.8	5.555556	-1.361(-1)	-2.241(-1)	-1.01(0)
0.9	10.526318	-7.205(-1)	-6.826(-1)	-3.383(0)
1.0	∞	-	-	-
1.1	-9.5238095	2.834(0)	1.216(0)	1.0476(1)
1.2	-4.5454545	-5.1177(-0)	-2.7018(0)	-1.7045(-0)

The values above suggest that the integrator and Adeboye[11] perform better than Fantula[10]. Therefore the integrator is a feasible numerical method.

CHAPTER FIVE

COMPUTER PROGRAMS

5.1 Computer Programs for the Problems Discussed in Chapter Four

```
PROGRAM PROB1 (input,output);

USES
  CRT;
CONST
  NOOFPTS = 50;
  PI = 3.141592654;
VAR
  EXACTY, X, Y {DUMMY VARIABLES} : ARRAY[0..NOOFPTS] OF REAL;
  STEP : REAL;
  INITX, FINALX : REAL;
  LASTI, I : INTEGER;
  COUNTER : REAL;
  CH : CHAR;

{****************************************************************** ********}

FUNCTION F(X, Y : REAL ) : REAL;
{THE DIFFERENTIAL EQUATION TO BE SOLVED IS OF THE FORM
 Y' = F(X, Y) }
  VAR SUPF : REAL;
BEGIN
  F := 1 + SQR(Y) ; {PROBLEM TO BE SOLVED}
END;

FUNCTION YEXACT( X : REAL ) : REAL;

{THIS FUNCTION GENERATES RESULTS FOR THE EXACT SOLUTION OF THE
 DIFFERENTIAL EQUATION UNDER CONSIDERATION (SEE FUNCTION F(X,Y)
}
VAR
  THETA : REAL;
BEGIN
  THETA := X + PI/4;
  YEXACT := SIN( THETA ) / COS( THETA );  { THE EXACT SOLUTION OF F(X,Y) }
END;

PROCEDURE DISPRES( N: INTEGER );
VAR
  PAGENO, LINENO, TOTLINE, J : INTEGER;
  ERROR : REAL;
BEGIN
  CLRSCR;
```

```
  TOTLINE := 25;
  WRITELN( ' X        EXACT     NEW       ERROR' );
  WRITELN( '          SOLUTION   SCHEME' );
  LINENO := 2;
  FOR J := 0 TO N DO
  BEGIN
    WRITE( X[J]:6:3,' ',YEXACT( X[J] ) :10:7,'  ', Y[J]:10:7, ' ' );
    EXACTY[ J ] := YEXACT( X[ J ] );
    ERROR := EXACTY[ J ] - Y[ J ] ;
    WRITELN( ERROR:10:7);
    LINENO := LINENO + 1;
    IF LINENO = TOTLINE - 1 THEN
    BEGIN
      CH := READKEY;
      CLRSCR;
      PAGENO := PAGENO + 1;
      LINENO := 1;
    END{IF};
  END;
END;
{************************************}
BEGIN {MAIN}
  CLRSCR;
  WRITE( 'PLEASE ENTER THE STEP LENGTH: ' );
  READLN( STEP );
  WRITE('PLEASE ENTER THE INITIAL VALUE OF X: ' );
  READLN( INITX );
  WRITE('PLEASE ENTER THE LAST VALUE OF X: ');
  READLN(FINALX);
  WRITE( 'PLEASE ENTER THE VALUE OF Y AT ',INITX:5:3,': ' );
  READLN( Y[0] );
  WRITE( 'PLEASE ENTER THE VALUE OF Y[1]: ' );
  READLN( Y[1] );

  X[0] := INITX;
  X[1] := INITX + STEP;
  COUNTER := INITX + STEP;
  I := 2;
  WHILE COUNTER <= FINALX DO
  BEGIN
    COUNTER := COUNTER + STEP;
    X[ I ] := X[ I - 1 ] + STEP;
    Y[ I ] := Y[ I - 2 ] * ( STEP * F( X[I - 1],Y[I-1] ) + Y[ I - 1 ] );
    Y[ I ] := Y[ I ] / ( Y[ I - 1 ] - ( STEP * F(X[I-1],Y[I-1]) ) );
    I := I + 1;
  END;
  LASTI := I - 1;
  DISPRES(LASTI);
  CH := READKEY;
```

```
END.

*************************************************************

PROGRAM PROB2 (input,output);

USES
  CRT;
CONST
  NOOFPTS = 50;
  PI = 3.141592654;
VAR
  EXACTY, X, Y {DUMMY VARIABLES} : ARRAY[0..NOOFPTS] OF REAL;
  STEP, MINH, MAXH, INCR : REAL;
  INITX, FINALX : REAL;
  X0, Y0 : REAL;
  K, LASTI, I : INTEGER;
  COUNTER : REAL;
  CH : CHAR;

{************************************************************* *******}

FUNCTION F(X, Y : REAL ) : REAL;
{THE DIFFERENTIAL EQUATION TO BE SOLVED IS OF THE FORM
 Y' = F(X, Y) }
  VAR SUPF : REAL;
BEGIN
  F := SQR(Y) ; {PROBLEM TO BE SOLVED}
END;

{*************************************************}

FUNCTION YEXACT( X : REAL ) : REAL;

{THIS FUNCTION GENERATES RESULTS FOR THE EXACT SOLUTION OF THE
 DIFFERENTIAL EQUATION UNDER CONSIDERATION (SEE FUNCTION F(X,Y)
}
BEGIN
  YEXACT := 1 / ( 1 - X ) ;  { THE EXACT SOLUTION OF F(X,Y) }
END;
{**********************************}
PROCEDURE DISPRES( N: INTEGER );
VAR
  PAGENO, LINENO, TOTLINE, J : INTEGER;
  ERROR : REAL;
BEGIN
  CLRSCR;
  TOTLINE := 25;
  WRITELN( ' X       EXACT     NEW       ERROR' );
```

```
  WRITELN( '          SOLUTION   SCHEME' );
  LINENO := 2;
  FOR J := 0 TO N DO
  BEGIN
    WRITE( X[J]:6:3,'  ');

    IF J = 10 THEN
      WRITE( 'INFINITY       INFINITY')
    ELSE
    BEGIN
      WRITE(YEXACT( X[J] ) :10:7,'   ');
      WRITE(Y[J]:10:7,'  ' );
    END;
    EXACTY[ J ] := YEXACT( X[ J ] );
    ERROR := EXACTY[ J ] - Y[ J ] ;

    IF J = 10 THEN
      WRITELN
    ELSE
      WRITELN( ERROR:10:7);

    EXACTY[ J ] := YEXACT( X[ J ] );
    LINENO := LINENO + 1;
    IF LINENO = TOTLINE - 1 THEN
    BEGIN
      CH := READKEY;
      CLRSCR;
      PAGENO := PAGENO + 1;
      LINENO := 1;
    END{IF};
  END;
END;
{**********************************}
BEGIN {MAIN}
  CLRSCR;
  WRITE( 'PLEASE ENTER THE STEP LENGTH: ' );
  READLN( STEP );
  WRITE('PLEASE ENTER THE INITIAL VALUE OF X: ' );
  READLN( INITX );
  WRITE('PLEASE ENTER THE LAST VALUE OF X: ');
  READLN(FINALX);
  WRITE( 'PLEASE ENTER THE VALUE OF Y AT ',INITX:5:3,': ' );
  READLN( Y[0] );
  WRITE( 'PLEASE ENTER THE VALUE OF Y[1]: ' );
  READLN( Y[1] );

  X[0] := INITX;
  X[1] := INITX + STEP;
  COUNTER := INITX + STEP;
```

```
  I := 2;
  WHILE COUNTER <= FINALX DO
  BEGIN
    COUNTER := COUNTER + STEP;
    X[ I ] := X[ I - 1 ] + STEP;
    Y[ I ] := Y[ I - 2 ] * ( STEP * F( X[I - 1],Y[I-1] ) + Y[ I - 1 ] );
    Y[ I ] := Y[ I ] / ( Y[ I - 1 ] - ( STEP * F(X[I-1],Y[I-1]) ) );
    I := I + 1;
  END;
  LASTI := I - 1;
  DISPRES(LASTI);
  CH := READKEY;
END
***************************************************************
PROGRAM PROB3 (input,output);

USES
  CRT;
CONST
  NOOFPTS = 50;
  PI = 3.141592654;
VAR
  EXACTY, X, Y {DUMMY VARIABLES} : ARRAY[0..NOOFPTS] OF REAL;
  STEP, MINH, MAXH, INCR : REAL;
  INITX, FINALX : REAL;
  X0, Y0 : REAL;
  K, LASTI, I : INTEGER;
  COUNTER : REAL;
  CH : CHAR;

FUNCTION F(X, Y : REAL ) : REAL;
{THE DIFFERENTIAL EQUATION TO BE SOLVED IS OF THE FORM
 Y' = F(X, Y) }
  VAR SUPF : REAL;
BEGIN
  F := X * SQR(Y) ; {PROBLEM TO BE SOLVED}
END;

{**************************************************}

FUNCTION YEXACT( X : REAL ) : REAL;

{THIS FUNCTION GENERATES RESULTS FOR THE EXACT SOLUTION OF THE
 DIFFERENTIAL EQUATION UNDER CONSIDERATION (SEE FUNCTION F(X,Y)
}
{VAR
  THETA : REAL;
}
BEGIN
```

```
{  THETA := X + PI/4;}
  YEXACT := 2 / ( 1 - SQR(X) ) ;  { THE EXACT SOLUTION OF F(X,Y) }
END;
{************************************}
PROCEDURE DISPRES( N: INTEGER );
VAR
  PAGENO, LINENO, TOTLINE, J : INTEGER;
  ERROR : REAL;
BEGIN
  CLRSCR;
  TOTLINE := 25;
  WRITELN( ' X       EXACT        NEW        ERROR' );
  WRITELN( '         SOLUTION     SCHEME' );
  LINENO := 2;
  FOR J := 0 TO N DO
  BEGIN
    WRITE( X[J]:6:3,'  ');

    IF J = 10 THEN
      WRITE( 'INFINITY      ')
    ELSE
      WRITE(YEXACT( X[J] ) :10:7,'   ');
    WRITE(Y[J]:10:7, ' ' );
    EXACTY[ J ] := YEXACT( X[ J ] );
    ERROR := EXACTY[ J ] - Y[ J ] ;

    IF J = 10 THEN
      WRITELN
    ELSE
      WRITELN( ERROR:10:7);

    LINENO := LINENO + 1;
    IF LINENO = TOTLINE - 1 THEN
    BEGIN
      CH := READKEY;
      CLRSCR;
      PAGENO := PAGENO + 1;
      LINENO := 1;
    END{IF};
  END;
END;
{************************************}
BEGIN {MAIN}
  CLRSCR;
  WRITE( 'PLEASE ENTER THE STEP LENGTH: ' );
  READLN( STEP );
  WRITE('PLEASE ENTER THE INITIAL VALUE OF X: ' );
  READLN( INITX );
  WRITE('PLEASE ENTER THE LAST VALUE OF X: ');
```

```
  READLN(FINALX);
  WRITE( 'PLEASE ENTER THE VALUE OF Y AT ',INITX:5:3,': ' );
  READLN( Y[0] );
  WRITE( 'PLEASE ENTER THE VALUE OF Y[1]: ' );
  READLN( Y[1] );

  X[0] := INITX;
  X[1] := INITX + STEP;
  COUNTER := INITX + STEP;
  I := 2;
  WHILE COUNTER <= FINALX DO
  BEGIN
    COUNTER := COUNTER + STEP;
    X[ I ] := X[ I - 1 ] + STEP;
    Y[ I ] := Y[ I - 2 ] * ( STEP * F( X[I - 1],Y[I-1] ) + Y[ I - 1 ] );
    Y[ I ] := Y[ I ] / ( Y[ I - 1 ] - ( STEP * F(X[I-1],Y[I-1]) ) );
    I := I + 1;
  END;
  LASTI := I - 1;
  DISPRES(LASTI);
  CH := READKEY;
END.
```

y = 1 + sqr(y), y(0) = 1

x	Exact Solution	New Scheme	Error
0.0000	1.0000000	1.0000000	0.0000000
0.0500	1.1053556	1.1053556	-0.0000000
0.1000	1.2230489	1.2234626	-0.0004138
0.1500	1.3560879	1.3565726	-0.0004847
0.2000	1.5084976	1.5095739	-0.0010763
0.2500	1.6857964	1.6871194	-0.0013230
0.3000	1.8957651	1.8980125	-0.0022474
0.3500	2.1497476	2.1526709	-0.0029232
0.4000	2.4649628	2.4695545	-0.0045917
0.4500	2.8688840	2.8753145	-0.0064305
0.5000	3.4082234	3.4184340	-0.0102106
0.5500	4.1693640	4.1854221	-0.0160580
0.6000	5.3318552	5.3604825	-0.0286273
0.6500	7.3404366	7.3981428	-0.0577062
0.7000	11.6813738	11.8388970	-0.1575232
0.7500	28.2382529	29.2415826	-1.0033297
0.8000	-68.4796678	-62.8918387	-5.5878292
0.8500	-15.4578961	-15.1335715	-0.3243246
0.9000	-8.6876295	-8.5768710	-0.1107586
0.9500	-6.0202997	-5.9633190	-0.0569807
1.0000	-4.5880378	-4.5521595	-0.0358783

y = Sqr(y), y(0) = 1

X	EXACT SOLUTION	NEW SCHEME	ERROR
0.0000	1.0000000	1.0000000	0.0000000
0.1000	1.1111111	1.1111111	0.0000000
0.2000	1.2500000	1.2500000	0.0000000
0.3000	1.4285714	1.4285714	0.0000000
0.4000	1.6666667	1.6666667	0.0000000
0.5000	2.0000000	2.0000000	0.0000000
0.6000	2.5000000	2.5000000	0.0000000
0.7000	3.3333333	3.3333333	0.0000001
0.8000	5.0000000	4.9999999	0.0000001
0.9000	10.0000000	9.9999995	0.0000005
1.0000	INFINITY	INFINITY	

y = Sqr(y), y(0) = 1

X	EXACT SOLUTION	NEW SCHEME	ERROR
0.0000	1.0000000	1.0000000	0.0000000
0.1000	1.1111111	1.1111111	0.0000000
0.2000	1.2500000	1.2500000	0.0000000
0.3000	1.4285714	1.4285714	0.0000000
0.4000	1.6666667	1.6666667	0.0000000
0.5000	2.0000000	2.0000000	0.0000000
0.6000	2.5000000	2.5000000	0.0000000
0.7000	3.3333333	3.3333333	0.0000001
0.8000	5.0000000	4.9999999	0.0000001
0.9000	10.0000000	9.9999995	0.0000005
1.0000	INFINITY	INFINITY	

y = x * sqr(y), y(0) = 2

X	EXACT SOLUTION	NEW SCHEME	ERROR
0.0000	2.0000000	2.0000000	0.0000000
0.1000	2.0202020	2.0202020	0.0000000
0.2000	2.0833333	2.0824742	0.0008591
0.3000	2.1978022	2.1957962	0.0020060
0.4000	2.3809524	2.3761833	0.0047691
0.5000	2.6666667	2.6570459	0.0096208
0.6000	3.1250000	3.1042747	0.0207253
0.7000	3.9215686	3.8733800	0.0481886
0.8000	5.5555556	5.4138502	0.1417054
0.9000	10.5263158	9.7919394	0.7343763
1.0000	INFINITY	85.7856389	
1.1000	-9.5238095	-12.3760542	2.8522447
1.2000	-4.5454545	-13.1279990	8.5825445

5.2 DISCUSSION OF THE RESULTS

The numerical values for problem one above suggest that the integrator is a feasible numerical method for treating initial value problems with discontinities/ singularities. We observe from the computational errors that smaller meshsize ,h, produce smaller global errors.

However, the integrator being two-step, is expected to use the values of y_n and y_{n+1} to compute y_{n+2} as an approximation to $y(x_{n+2})$. To achieve this we simply generate the value of y_{n+1} using the exact solution. The integrator couverges rapidly when used to solve certain initial value problems with singularities.

The numerical values as shown in the results of problem two indicate also that the integrator is a good numerical methods. The results show the exceedingly high performcane of the integrator. The integrator gives accurate results nearly as good as the theoretical results.

Also in problem three we constrast the results and observe that the integrator performs well in this class of initial value problems therefore the integrator is well suited for initial value problems with discontinuities or singularities.

5.3 SUMMMARY , CONCLUSION AND RECOMMENDATION

5.3.1 SUMMARY AND CONCLUSION

We shall conclude this project by summarising the details of the previous chapters. In chapter one, we discussed the general historical background of the subject differential equation. In chapter one also we give some discussions about the development of some important linear multi-step methods such as Euler's rule, Mid-point rule, trapezoidal rule, Adams-Moulton methods etc. We also discussed the derivation of some finite difference schemes for solving partial differential equations.

Chapter two is mainly the literature review on the treatment of singular and discontinuous initial value problems. The overview of some methods of treating singular and discontinuous system such as non- polynomial methods, inverse polynomial, explicit convergent one-step method, and a fifth order L-stable numerical methods were made.

A new scheme for treating singular and discontinuous systems was established in chapter three. The integrator is zero stable and consistent. Hence, it is convergent. The new scheme is proposed to cope with singular and discontinuous intial value problems. It may not cope with stiff and oscillatory differential equation.

Some numerical experiments were performed in chapter four using the new integrator. We also compared the performance of the new integrator with the theorical solutions. The integrator converges rapidly for certain initial value problems.

Finally some computer programmes were written to solve the initial value problems discussed in chapter four. The results of the programmes as contrasted with the theoritical solutions show that the integrator is a good numerical method.

5.3.2 RECOMMENDATION

The area of mathematical formulation of physical phenomena in electical engineering, simulation, control theory and economics often gives or leads to an initial value problem of the form $y' = f(x,y)$, $y(0) = y_0$. The fundamental concern is always the computation or solution of such problems. However, most of the conventional integrator formulas, i.e linear multistep methods perform very inefficiently in the treatment of a singularity. In order to circumvent this problem it is important to provide alternative strategies so as to establish algorithms which will perform well in the treatment of singularities. To achieve this, it is recommendable to research into the subject of this research work and earlier works.

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