IMPLICIT MULTI – DERIVATIVE, LINEAR MULTI – STEP METHODS FOR NUMERICAL SOLUTION OF FIRST ORDER ORDINARY DIFFERENTIAL EQUATIONS

BY

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CERTIFICATION

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DEDICATION

This thesis is dedicated to God Almighty; the source of knowledge and wisdom.

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ABSTRACT

This work considered the development, analysis and implementation of a class of implicit multi – derivative linear multi – step methods of the form:

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = \sum_{i=1}^{l} h^i \sum_{j=0}^{k}\beta_{ij} y^i_{n+j};\ \alpha_k = +1$$

with local truncation error T_{n+k} defined as

$$T_{n+k} = \sum_{j=0}^{k}\alpha_j y_{n+j} - \sum_{i=1}^{l} h^i \sum_{j=0}^{k}\beta_{ij} y^i_{n+j}$$

for the solution of initial value problems of First Order Ordinary Differential Equations of the form:

$$y' = f(x,y), y(x_0) = y_0, a \le x \le b$$

The development of the methods adopts the Taylor Series expansion of the functions y_{n+j}, y'_{n+j} and y''_{n+j}. Accuracy of order P is then imposed on T_{n+k}. The resulting equations are solved for parameters α_j's and β_{ij}'s to generate the required methods (schemes).

The analysis of the basic properties of the methods such as the order of accuracy, consistency, convergence and A-stability were carried out. The results showed that the methods are accurate and absolutely stable (A – stable).

The methods are implemented on a digital computer adopting FORTRAN programming language. The programmes are used to solve some sample first order initial value problems. The results showed that the schemes are accurate and convergent. The developed methods are compared with some standard linear multi-step methods like Adams Moulton's and Addison's methods, for which the results showed that the methods are accurate and efficient.

CHAPTER ONE

INTRODUCTION

1.1 Preamble

Differential equations occur in connection with the mathematical description of problems that are encountered in various branches of science like Mechanics, Chemistry, Biology and Economics. Consequently, it constitutes a large and very important aspect of today's mathematics. The problems that give rise to differential equations include:

- Determination of charge or current in an electric circuit.
- Conduction of heat in a rod or in a slab.
- Determination of motion of a projectile, rocket, satellite or planet.
- Rate of decomposition of a radioactive substance or the rate of growth of human or animal populations.
- Studying of the chemical reactions of substances, just to mention a few.

Though these problems exist by theory or principle, their mathematical analysis give rise to differential equations, because the objects involved obey certain physical and chemical laws involving rates of change (Auzinger; *et al,* 1990; Courant F. 2007; Ross, 1989). The resulting differential systems may be ordinary or partial differential equations. It is ordinary differential equation when the dependent variable y is a function of a single independent variable x but when y is a function of two or more independent variables, then a partial differential equation evolve. Only a few of these differential equations can be solved analytically, this reason gave the search for numerical approximation.

1.2 Initial Value Problems of Ordinary Differential Equations

Ordinary differential equations (ODEs) can be classified into two: Initial Value Problem (IVP) or Boundary Value Problem (BPV) depending upon the given condition. A differential equation together with initial condition prescribed at one point is called IVP. For example, the differential equation

$$y^{1} = x + y,\ y(0) = 1$$

with condition prescribed at one point x =0 is called IVP.

A differential equation together with conditions specified at two ends is called BVP. For example, the differential equation

$$y^{1} = x + 2y,\ y(0) = 1, y(1) = 0$$

with condition prescribed at two points x=0 and x=1 is called BVP

Thus, a differential equation of the form

$$y' = f(x,y), y(x_0) = y_0, a \le x \le b \qquad \text{...1.1}$$

is a first order IVP where f is assumed to be Lipschitz continuous (Gonzalez *et al*; 2002)

1.3 Basic Concepts and Principles

This chapter is concerned in defining some concepts and principles that will be used in this thesis.

1.3.1 Linear Multistep Method

A Linear Multi-step Method (LMM) for numerical solution of first order ordinary differential equations of the kind (1.1) is a computational method of the form:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j y'_{n+j} \qquad \text{...1.2}$$

for approximating y_n at the successive points (x_n, y_n), where α_j and β_j are constants to be determined (Auzinger, *et al;* 1993).

In this study we consider the development of methods for which k=1 and 2 respectively. In a single- step method like Runge-Kutta method which is self starting, the value of y_{n+1} at x_{n+1} depends only on y_n while a multistep methods like Adam Bathsforth , Adam Moulton's method and the proposed methods, to compute the value of y_{n+1} at x_{n+1} several other previous values of y, such as y_n, y_{n-1}, y_{n-2}...... are required. The order of the method depends on how many previous steps were used to get each new value of y (Auzinger *et al*; 1996; Ostermann and Thalhammer, 2002).

1.3.2 Explicit and Implicit Linear Multistep Method

A linear multistep method of the form (1.2) can either be explicit or implicit, Eqn (1.2) is explicit when β_k =0, this makes it possible to determine the current value of y_{n+j} directly from the previous steps values; y_{n+j}, f_{n+j} , j=0(1)k-1 that have already been found. Equation (1.2) is implicit when $\beta_k \neq 0$. As can be seen, the unknown value y_{n+k} is also present on the right hand side. There is therefore a need to generate a good initial value $y^{(0)}_{n+k}$ for y_{n+k} together with the previous values y_{n+j}, f_{n+j} , j=0(1)k-1 which are then adopted for calculation in the formula

$$y_{n+k} = \sum_{i=j=0}^{k-1}\alpha_i y_{n+j} + h\sum_{j=0}^{k}\beta_j f_{n+j} \qquad \text{.........................1.3}$$

According to Fatunla (1988), we shall see that implicit methods are more accurate and have large interval of absolute stability when compared with explicit methods.

1.3.3 Stiff Ordinary Differential Equations

A differential equation defined by equation (1.1) is said to be stiff if its Lipstchitz constant

$$L = \left| \delta f / \delta y \right| \gg 1$$

Stiff IVPs are frequent occurrencies in the mathematical formulation of physical situations in control theory and mass action kinetics where processes with widely varying time constants are usually considered.

Certain types of problems can be characterized as stiff;

(i) problems of the form

$$y^{1} = ky + f(t) \text{ where } |k| \text{ is large}$$

(ii) systems of the form

$y^{1} = ky + f(t)$ where k is a square matrix having at least one eigenvalue $|l|$ large

(iii) systems of the form

$y^{1} = f(y,t)$ is with the Jacobian of f having at least one eigen value $|m|$ large

The behaviour of numerical methods on stiff problems can be analyzed by applying this methods to the test equation

$$y^{1} = \Lambda y$$

the solution of this equation is

$$y(t) = e^{\Lambda t}.$$

This solution approaches zero as t →∞ when Re λ < 0. If the numerical method also exhibit this behaviour, the method is said to be A-stable and adequate for solving stiff problems.

1.3.4 Discretization and Step Size

This is a principle in which an approximation to unknown variable y is sought on certain discrete point set.

$\{x_i \mid a = x_0 < x_1 < x_2 < \ldots\ldots < x_n = b\}$

while the parameter $h = x_{i+1} - x_i$, $i = 0(1)n-1$

is the step size or mesh size.

1.3.5 Multiderivative Method

This is a method which uses not only the function y and its first derivative but also its higher derivatives. Thus it involves more analytical properties of the differential equation by way of more of the derivative properties of y (Eder and Kurlinger, 2001; Bakaev and Ostermann, 2002; Palencia,, 1993).

1.4 Existing Linear Multistep Methods

Various approximation methods for solving first order ordinary differential equations of the form (1.1) have been developed, they include Adams Moulton and Adams Bathforth's Linear Multi-step Methods defined by (1.2), Gear's Backward Differentiation Method (BDF) and Addison linear multi-step method, to mention a few.

These methods, though multi-step include only the first order derivative property of the differential equation. This study wants to include more derivative properties of the differential equation into the existing linear multi-step method (1.2) for numerical solution of ordinary differential equations of type (1.1) in the hope that it will have better accuracy, stability and efficiency.

Consequently, a class of implicit multi derivative formula of the form.

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = \sum_{i=1}^{l} h^i \sum_{j=0}^{k} \beta_{ij} y^{i}_{n+j}; \ \alpha_k = +1 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 1.4$$

involving more derivative properties of the differential equation is proposed for the solution of both non – stiff and stiff initial value problems of Ordinary Differential Equations (O.D.Es). It is hopeful that it will be more superior in accuracy and stability than the existing linear multi-step methods.

1.5 Research Aim and Objectives

1.5.1 Research Aim

The aim of this study is to improve on the accuracy and stability of existing linear multi-step methods.

1.5.2 Research objectives

The purpose of this study is to:

(i) derive a class of implicit multi-derivative linear multi-step methods which are capable of solving non – stiff and stiff initial value problems of first order ordinary differential equations.

(ii) examine the basic properties such as accuracy, consistency, zero – stability, convergence, absolute stability and its region.

(iii) apply the methods to solve some non – stiff and stiff first order IVP of ODEs.

1.6 Research Methodology

The methods adopt Taylor's series expansion of y_{n+j}, j=0(1)k in the truncation error associated with the methods, defined as:

$$T_{n+k} = \sum_{j=0}^{k} \alpha_j y_{n+j} - \sum_{i=1}^{l} h^i \sum_{j=0}^{k} \beta_{ij} y^i_{n+j}$$

Accuracy of order P is imposed on T_{n+k} and the resulting equations are solved for parameters $\alpha_j^{'s}$ and $\beta_{ij}^{'s}$ to generate the required methods for step numbers k = 1 and 2 respectively.

The basic properties of the methods such as accuracy, consistency, convergence, stability and its region are analyzed using Dalhquist stability model test equation and Boundary locus method as described in Lambert (1973) and Fatunla (1988).

The methods are implemented on a digital computer adopting Fortran programming language. Some sample non – stiff and stiff initial value problems of ODE are solved.

1.7 Expected Contribution To Knowledge

The findings of this study,(has reported in Chapter Four have produced a new class of implicit linear multi-step methods of improved accuracy and stability for solution of non – stiff and stiff initial value problems of ordinary differential equations.

CHAPTER TWO

DERIVATION OF THE METHODS

2.0 Introduction

Linear multistep methods of the form (1.2) can be classified into explicit and implicit methods (Lambert, 1973). The method is explicit when $\beta_k = 0$ and implicit when $\beta_k \neq 0$. In this study, we are concerned with the development, analysis and implementation of a family of implicit multiderivative linear multistep methods. That is, methods for which $\beta_k \neq 0$. To achieve this, consider the local truncation error formula (1.5) to determine parameters α_j's and β_{ij}'s of the formula (1.4) for step numbers k=1 and 2.

Consequently, it is assumed that the local truncation error T_{n+k} for step application of the formula to problem (1.1) can be defined as:

$$T_{n+k} = \sum_{j=0}^{k} \alpha_j y_{n+j} - \sum_{i=1}^{l} h^i \sum_{j=0}^{k} \beta_{ij} y^i_{n+j} \qquad \text{.........................2.1}$$

where l is the order of the derivative of y_{n+j}

Adopting Taylors series expansion of variables y^i_{n+j}, $j = 0(1)$, and $i = 0(1)l$. given as:

$$y^i_{n+j} = \sum_{r=0}^{\infty} \frac{(\mathrm{jh})^r y^{r+i}}{r!}, \ \mathrm{j=1(1)m}$$

in equation (2.1) and combine terms in equal powers of h, we have

$$T_{n+k} = C_0 y_n + C_1 h y'_n + C_2 h^2 y''_n + ...C_p h^p y^p + ...(h^{p+1})$$

where

$$C_p = \frac{1}{p!}\sum_{j=1}^{k} j^p \alpha_j - \frac{1}{(p-1)!}\sum_{j=1}^{k} j^{(p-1)}\beta_{1j} - \frac{1}{(p-2)!}\sum_{j=1}^{k} j^{(p-2)}\beta_{2j}$$

2.2 DERIVATIONS

2.2.1 One – Step First Derivative Method

Setting k=1,l=1 in equation 1.4 gives

$$\alpha_0 y_n + \alpha_1 y_{n+1} = h\beta_{10} y'_n + h\beta_{11} y'_{n+1} \quad \text{...........................2.3}$$

with local truncation error.

$$T_{n+1} = \alpha_0 y_n + \alpha_1 y_{n+1} - h\beta_{10} y'_n - h\beta_{11} y'_{n+1} \quad \text{.....................2.4}$$

The Taylor's expansion of

$$y_{n+1} = y_n + hy'_n + \frac{h^2 y''}{2!} + \frac{h^3 y'''}{3!} + \ldots\ldots + 0(h^4) \quad \text{................2.5}$$

and

$$y'_{n+1} = y'_n + hy''_n + \frac{h^2 y'''}{2!} + \frac{h^3 y''''}{3!} + \ldots\ldots + 0(h^4) \quad \text{................2.6}$$

Substituting these into equation (2.4) and combine terms in equal powers of h, we have

$$T_{n+1} = C_0 y_n + C_1 h y'_n + C_2 h^2 y''_n + C_3 h^3 y'''_n + \ldots + 0(h^4)$$

where

$$C_0 = \alpha_0 + \alpha_1$$
$$C_1 = \alpha_1 - \beta_{10} - \beta_{11}$$
$$C_2 = \tfrac{1}{2}\alpha_1 - \beta_{11}$$
$$C_3 = \tfrac{1}{6}\alpha_1 - \tfrac{1}{2}\beta_{11}$$

Imposing accuracy of order 2 on T_{n+1}, to have $C_0 = C_1 = C_2 = 0$ and $T_{n+1} = 0(h^3)$.

That is,

$$\alpha_0 + \alpha_1 = 0$$

$$\alpha_1 - \beta_{10} - \beta_{11} = 0$$

$$\tfrac{1}{2}\alpha_1 - \beta_{11} = 0$$

$$C_3 = \tfrac{1}{6}\alpha_1 - \tfrac{1}{2}\beta_{11} \neq 0$$

Solving this set of equations with $\alpha_1 = 1$, we obtain

$$\alpha_0 = -1, \beta_{10} = \tfrac{1}{2} \text{ and } \beta_{11} = \tfrac{1}{2}$$

Substituting these values into equation (2.3) and simplifying to obtain a one-step first derivative method of the form:

$$y_{n+1} = y_n + \frac{h}{2}\left(y'_{n+1} + y'_n\right) \qquad \ldots\ldots\ldots \qquad (2.7)$$

which coincides with the Trapezoidal method (Lambert, 1973).

2.2.2 One – Step Second Derivative Method

Setting $k = 1, l = 2$ in (1.4) gives

$$\alpha_0 y_n + \alpha_1 y_{n+1} = h\left[\beta_{10} y'_n + \beta_{11} y'_{n+1}\right] + h^2\left[\beta_{20} y''_n + \beta_{21} y''_{n+1}\right] \qquad \ldots\ldots\ldots \qquad (2.8)$$

with local truncation error

$$T_{n+1} = \alpha_0 y_n + \alpha_1 y_{n+1} - h\left[\beta_{10} y'_n + \beta_{11} y'_{n+1}\right] - h^2\left[\beta_{20} y''_n + \beta_{21} y''_{n+1}\right] \ldots\ldots\ldots \qquad (2.9)$$

Adopting the Taylor's series expansion of y_{n+1} and y^1_{n+1} as in equations (2.5) and (2.6) respectively and

$$y''_{n+1} = y''_n + hy'''_n + \frac{h^2 y^{iv}}{2!} + \frac{h^3 y^{v}}{3!} + \ldots\ldots + 0(h^4) \qquad \ldots\ldots\ldots\ldots\ldots\ldots (2.10)$$

in (2.9), combining terms in equal powers of h gives

$$T_{n+1} = C_0 y_n + C_1 h y'_n + C_2 h^2 y''_n + C_3 h^3 y'''_n + C_4 h^4 y^{iv}_n + 0\left(h^5\right)$$

where,

$$C_0 = \alpha_0 + \alpha_1$$

$$C_1 = \alpha_1 - \beta_{10} - \beta_{11}$$

$$C_2 = \frac{\alpha_1}{2} - \beta_{11} - \beta_{20} - \beta_{21}$$

$$C_3 = \frac{\alpha_1}{6} - \frac{\beta_{11}}{2} - \beta_{21}$$

$$C_4 = \frac{\alpha_1}{24} - \frac{\beta_{11}}{6} - \frac{\beta_{21}}{2}$$

$$C_5 = \frac{\alpha_1}{120} - \frac{\beta_{11}}{24} - \frac{\beta_{21}}{6}$$

Imposing accuracy of order 4 on T_{n+1}, to have $C_0 = C_1 = C_2 = C_3 = C_4 = 0$ and

$T_{n+1} = 0(h^5)$.

Consequently, we obtain the following system of linear equations

$$\alpha_0 + \alpha_1 = 0$$

$$\alpha_1 - \beta_{10} - \beta_{11} = 0$$

$$\frac{1}{2}\alpha_1 - \beta_{11} - \beta_{20} - \beta_{21} = 0$$

$$\frac{1}{6}\alpha_1 - \frac{1}{2}\beta_{11} - \beta_{21} = 0$$

$$\frac{1}{24}\alpha_1 - \frac{1}{6}\beta_{11} - \frac{1}{2}\beta_{21} = 0$$

$$\frac{\alpha_1}{120} - \frac{\beta_{11}}{24} - \frac{\beta_{21}}{6} \neq 0$$

Solving this set of equations with $\alpha_1 = 1$ gives

$\alpha_0 = -1$, $\beta_{10} = \frac{1}{2}$, $\beta_{11} = \frac{1}{2}$, $\beta_{20} = +\frac{1}{12}$ and $\beta_{21} = -\frac{1}{12}$.

Substituting these values into equation (2.8) and simplifying to obtain a one step linear multiderivative multistep formula

$$y_{n+1} = y_n + \frac{h}{2}\left[y'_{n+1} + y'_n\right] - \frac{h^2}{12}\left[y''_{n+1} - y''_n\right] \quad \ldots\ldots \quad (2.11)$$

2.2.3 Two – Step First Derivative Linear Multi-step Method

Setting $k = 2, l = 1$ in (1.4), gives

$$\alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} = h\left[\beta_{10} y'_n + \beta_{11} y'_{n+1} + \beta_{12} y'_{n+2}\right] \quad \ldots\ldots \quad (2.12)$$

with local truncation error

$$T_{n+2} = \alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} - h\left[\beta_{10} y'_n + \beta_{11} y'_{n+1} + \beta_{12} y'_{n+2}\right] \quad \ldots\ldots \quad (2.13)$$

Adopting the Taylor's series expansion of y_{n+1}, y'_{n+1}, y_{n+2} and y'_{n+2} as given in equations (2.5), (2.6), (2.14) and (2.15) in equation (2.13)

$$y_{n+2} = y_n + 2hy'_n + \frac{4h^2 y''}{2!} + \frac{8h^3 y'''}{3!} + \ldots\ldots + 0(h^4) \quad \ldots\ldots\ldots \ldots\ldots \quad (2.14)$$

$$y'_{n+2} = y'_n + 2hy''_n + \frac{4h^2 y'''}{2!} + \frac{8h^3 y''}{3!} + \ldots\ldots + 0(h^4) \quad \ldots\ldots\ldots\ldots\ldots\ldots (2.15)$$

and combine terms of equal power of h we have ,

$$T_{n+2} = C_0 y_n + C_1 hy'n + C_2 h^2 y''n + C_3 h^3 y'''n + 0(h^4)$$

where

$$C_0 = \alpha_0 + \alpha_1 + \alpha_1$$

$$C_1 = \alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12}$$

$$C_2 = \frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12}$$

$$C_3 = \frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{12}$$

$$C_4 = \frac{\alpha_1}{24} + \frac{2}{3}\alpha_2 - \frac{\beta_{11}}{6} - \frac{4}{3}\beta_{12}$$

$$C_5 = \frac{1}{120}\alpha_1 - \frac{4}{15}\alpha_2 + \frac{1}{24}\beta_{11} + \frac{2}{3}\beta_{12}$$

Imposing accuracy of order 4 on T_{n+2}, we have $C_0 = C_1 = C_2 = C_3 = C_4 = 0$ and $T_{n+2} = 0(h^5)$

That is,

$$\alpha_0 + \alpha_1 + \alpha_1 = 0$$

$$\alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12} = 0$$

$$\frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12} = 0$$

$$\frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{21} = 0$$

$$\frac{\alpha_1}{24} + \frac{2}{3}\alpha_2 - \frac{\beta_{11}}{6} - \frac{4}{3}\beta_{21} \neq 0$$

$$\frac{\alpha_1}{120} + \frac{4}{15}\alpha_2 - \frac{\beta_{11}}{24} - \frac{2}{3}\beta_{21} \neq 0$$

Solving this set of equations with $\alpha_2 = 1$gives

$$\alpha_0 = -1,\ \alpha_1 = 0,\ \beta_{10} = \tfrac{1}{3},\ \beta_{11} = \tfrac{4}{3} \text{ and } \beta_{12} = \tfrac{1}{3}$$

Substituting these values into equation (2.12) and simplifying we obtain a two-step first derivative formula of the form:

$$y_{n+2} = y_n + \frac{h}{3}\left(y'_{n+2} + 4y'_{n+1} + y'_n\right) \qquad \ldots\ldots\ldots \qquad (2.16)$$

which coincides with Simpson's one – third rule (Lambert, 1973).

2.4 Two – Step Second Derivative Linear Multi-step Method

Setting $k=2, l=2$ in (1.4) gives

$$\alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} = h[\beta_{10} y'_n + \beta_{11} y'_{n+1} + \beta_{12} y'_{n+2}] + h^2[\beta_{20} y''_n + \beta_{21} y''_{n+1} + \beta_{22} y''_{n+2}] \quad \ldots (2.17)$$

with local truncation error:

$$T_{n+2} = \alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} - h[\beta_{10} y'_n + \beta_{11} y'_{n+1} + \beta_{12} y'_{n+2}] - h^2[\beta_{20} y''_n + \beta_{21} y''_{n+1} + \beta_{22} y''_{n+2}]$$

.... (2.18)

Adopting the Taylor's series expansion of y_{n+1}, y'_{n+1}, y_{n+2} and y'_{n+2} as in equations (2.5), (2.6), (2.14) and (2.15) in equation (2.18) and combine terms in equal powers of h we obtain

$$T_{n+2} = C_0 y_n + C_1 h y' n + C_2 h^2 y'' n + C_3 h^3 y''' n + \ldots.. + C_7 h^7 y''' n + 0(h^8)$$

where

$$C_0 = \alpha_0 + \alpha_1 + \alpha_2$$

$$C_1 = \alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12}$$

$$C_2 = \frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12} - \beta_{20} - \beta_{21} - \beta_{22}$$

$$C_3 = \frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{12} - \beta_{21} - 2\beta_{22}$$

$$C_4 = \frac{\alpha_1}{24} + \frac{2\alpha_2}{3} - \frac{\beta_{11}}{6} - \frac{4}{3} - \beta_{12} - \frac{\beta_{21}}{2} - 2\beta_{22}$$

$$C_5 = \frac{1}{3}\left(\frac{\alpha_1}{40} + \frac{4}{15}\alpha_2 - \frac{1}{8}\beta_{11} - 2\beta_{12} - \frac{1}{2}\beta_{21} - 4\beta_{22}\right)$$

$$C_6 = \frac{1}{3}\left(\frac{\alpha_1}{240} + \frac{4}{15}\alpha_2 - \frac{1}{40}\beta_{11} - \frac{4}{5}\beta_{12} - \frac{1}{8}\beta_{21} - 2\beta_{22}\right)'$$

$$C_7 = \frac{1}{3}\left(\frac{\alpha_1}{1680} + \frac{8}{105}\alpha_2 - \frac{1}{240}\beta_{11} - \frac{4}{15}\beta_{12} - \frac{1}{40}\beta_{21} - \frac{4}{5}\beta_{22}\right)$$

$$C_8 = \frac{1}{40320}(\alpha_1 + 256\alpha_2) - \frac{1}{5040}(\beta_{11} + 128\beta_{12}) - \frac{1}{720}(\beta_{21} + 64\beta_{22})$$

Imposing accuracy of order 7 on T_{n+2}, to have

$C_0 = C_1 = C_2 = C_3 = C_4 = C_5 = C_6 = C_7 = 0$, and T_{n+2}=0(h^8)

That is,

$$\alpha_0 + \alpha_1 + \alpha_2 = 0$$

$$\alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12} = 0$$

$$\frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12} - \beta_{20} - \beta_{21} - \beta_{22} = 0$$

$$\frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{12} - \beta_{21} - 2\beta_{22} = 0$$

$$\frac{\alpha_1}{24} + \frac{2\alpha_2}{3} - \frac{\beta_{11}}{6} - \frac{4}{3}\beta_{12} - \frac{\beta_{21}}{2} - 2\beta_{22} = 0$$

$$\frac{\alpha_1}{40} + \frac{4}{5}\alpha_2 - \frac{1}{8}\beta_{11} - 2\beta_{12} - \frac{1}{2}\beta_{21} - 4\beta_{22} = 0$$

$$\frac{\alpha_1}{240} + \frac{4}{15}\alpha_2 - \frac{1}{40}\beta_{11} - \frac{4}{5}\beta_{12} - \frac{1}{8}\beta_{21} - 2\beta_{22} = 0$$

$$\frac{\alpha_1}{1680} + \frac{8}{105}\alpha_2 - \frac{1}{240}\beta_{11} - \frac{4}{15}\beta_{12} - \frac{1}{40}\beta_{21} - \frac{4}{5}\beta_{22} = 0$$

Solving this set of equations gives

$$\begin{array}{lll} \alpha_0 = 1 & \beta_{10} = -3/8 & \beta_{20} = -1/24 \\ \alpha_1 = -2 & \beta_{11} = 0 & \beta_{21} = 1/3 \\ \alpha_2 = 1 & \beta_{12} = 3/8 & \beta_{22} = -1/24 \end{array}$$

Substituting these values into equation (2.17) and simplifying we obtain a two-step second derivative formula of the form:

$$y_{n+2} = 2y_{n+1} - y_n + \frac{3h}{8}(y'_{n+2} - y'_n) - \frac{h^2}{24}(y''_{n+2} - 8y''_{n+1} + y''_n) \qquad \text{........ (2.19)}$$

CHAPTER THREE

BASIC PROPERTIES OF THE METHODS

A good numerical method for solution of ordinary differential equations is required to be accurate, consistent, zero-stable, convergent and absolutely-stable.

To ensure that the new methods have these basic properties, the properties are investigated.

3.1 Order of Accuracy and Error Constant of the Methods

Errors are often generated when numerical formula is used to solve a differential equation. These errors occur as a result of using approximate values of function y, coupled with numerical truncation. The magnitude of the error determines the degree of accuracy of the schemes. If the magnitude is adequately small, the method is said to be accurate, otherwise it is inaccurate (Babatola and Ademiluyi, 2007). Its effect on numerical solution is to make it deviate significantly from the exact solution, which can make the solution unstable.

According to Lambert (1973) and Fatunla (1988), a linear multi step method is said to be of order P if the order of the local truncation error T_{n+k} is P.

3.1.1 One-Step First Derivative Method

For the One-Step First Derivative Method (2.7) the local truncation error

$$T_{n+1} = C_0 y_n + C_1 h y'_n + C_2 h^2 y''_n + C_3 h^3 y'''_n + C_4 h^4 y^{iv}_n + 0(h^5)$$

where

$$\left.\begin{aligned} C_0 &= \alpha_0 + \alpha_1 \\ C_1 &= \alpha_1 - \beta_{10} - \beta_{11} \\ C_2 &= \tfrac{1}{2}\alpha_1 - \beta_{11} \\ C_3 &= \tfrac{1}{6}\alpha_1 - \tfrac{1}{2}\beta_{11} \end{aligned}\right\} \qquad \text{..................3.1}$$

with

$\alpha_0 = -1, \beta_{10} = \frac{1}{2}$ and $\beta_{11} = \frac{1}{2}$

Substituting these values into equation 3.1 to have

$$C_0 = -1 + 1 = 0$$

$$C_1 = 1 - \frac{1}{2} - \frac{1}{2} = 0$$

$$C_2 = \frac{1}{2} - \frac{1}{2} = 0$$

$$C_3 = \frac{1}{6} - \frac{1}{4} = -\frac{1}{12} \neq 0$$

implying that, $C_0 = C_1 = C_2 = 0$, $C_3 = -\frac{1}{12} \neq 0$

hence method (2.7) is of order 2 with error constant $C_3 = -\frac{1}{12}$

3.1.2 One-Step Second Derivative Method

For the one-step second derivative method (2.11) the local truncation error

$$T_{n+1} = C_0 y_n + C_1 h y'_n + C_2 h^2 y''_n + C_3 h^3 y'''_n + C_4 h^4 y^{iv}_n + 0(h^5)$$

where

$$\left.\begin{aligned}
C_0 &= \alpha_0 + \alpha_1 \\
C_1 &= \alpha_1 - \beta_{10} - \beta_{11} \\
C_2 &= \frac{\alpha_1}{2} - \beta_{11} - \beta_{20} - \beta_{21} \\
C_3 &= \frac{\alpha_1}{6} - \frac{\beta_{11}}{2} - \beta_{21} \\
C_4 &= \frac{\alpha_1}{24} - \frac{\beta_{11}}{6} - \frac{\beta_{21}}{2} \\
C_5 &= \frac{\alpha_1}{120} - \frac{\beta_{11}}{24} - \frac{\beta_{21}}{6}
\end{aligned}\right\} \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad 3.2$$

with

$\alpha_0 = -1$, $\beta_{10} = \frac{1}{2}$, $\beta_{11} = \frac{1}{2}$, $\beta_{20} = +\frac{1}{12}$ and $\beta_{21} = -\frac{1}{12}$.

Substituting these values into equation (3.2) gives

$$C_0 = -1 + 1 = 0$$

$$C_1 = 1 - \frac{1}{2} - \frac{1}{2} = 0$$

$$C_2 = \frac{1}{2} - \frac{1}{2} - \frac{1}{12} + \frac{1}{12} = 0$$

$$C_3 = \frac{1}{6} - \frac{1}{4} + \frac{1}{12} = 0$$

$$C_4 = \frac{1}{24} - \frac{1}{12} + \frac{1}{24} = 0$$

$$C_5 = \frac{1}{120} - \frac{1}{48} + \frac{1}{72} = \frac{1}{720} \neq 0$$

Implying that $C_0 = C_1 = C_2 = C_3 = C_4 = 0$, $C_5 = \frac{1}{720} \neq 0$

Hence, method (2.11) is of order 4 with error constant $C_5 = \frac{1}{720}$

3.1.3 Two-Step First Derivative Method

For the Two-Step First Derivative Method (2.16) the local truncation error

$$T_{n+2} = C_0 y_n + C_1 h y'_n + C_2 h^2 y''_n + C_3 h^3 y'''_n + C_4 h^4 y^{iv}_n + 0\left(h^5\right)$$

where

$$\left.\begin{aligned}
C_0 &= \alpha_0 + \alpha_1 + \alpha_2 \\
C_1 &= \alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12} \\
C_2 &= \frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12} \\
C_3 &= \frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{12} \\
C_4 &= \frac{\alpha_1}{24} + \frac{2}{3}\alpha_2 - \frac{\beta_{11}}{6} - \frac{4}{3}\beta_{12} \\
C_5 &= \frac{1}{120}\alpha_1 - \frac{4}{15}\alpha_2 + \frac{1}{24}\beta_{11} + \frac{2}{3}\beta_{12}
\end{aligned}\right\} \qquad \ldots\ldots\ldots\ldots\ldots \quad 3.3$$

with

$\alpha_0 = -1$, $\alpha_1 = 0$, $\beta_{10} = \frac{1}{3}$, $\beta_{11} = \frac{4}{3}$ and $\beta_{12} = \frac{1}{3}$

Substituting these values into equation (3.3) we have

$$C_0 = -1 + 0 + 1 = 0$$

$$C_1 = 0 - 2 - \frac{1}{3} - \frac{4}{3} - \frac{1}{3} = 0$$

$$C_2 = 0 + 2 - \frac{4}{3} - \frac{2}{3} = 0$$

$$C_3 = 0 + \frac{4}{3} - \frac{4}{6} - \frac{2}{3} = 0$$

$$C_4 = 0 + \frac{2}{3} - \frac{4}{18} - \frac{4}{9} = 0$$

$$C_5 = 0 - \frac{4}{15} - \frac{4}{72} - \frac{2}{9} = \frac{1}{90}$$

Implying that $C_0 = C_1 = C_2 = C_3 = C_4 = 0$, and $C_5 = \frac{1}{90} \neq 0$

Hence, method (2.16) is of order 4 with error constant $C_5 = \frac{1}{90}$

3.1.4 Two-Step Second Derivative Method

For the Two-Step Second Derivative Method (2.19) the local truncation error

$$T_{n+2} = C_0 y_n + C_1 h y' n + C_2 h^2 y'' n + C_3 h^3 y''' n + \ldots + C_7 h^7 y''' n + 0(h^8)$$

where

$$\left.\begin{aligned}
C_0 &= \alpha_0 + \alpha_1 + \alpha_2 \\
C_1 &= \alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12} \\
C_2 &= \frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12} - \beta_{20} - \beta_{21} - \beta_{22} \\
C_3 &= \frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{12} - \beta_{21} - 2\beta_{22} \\
C_4 &= \frac{\alpha_1}{24} + \frac{2\alpha_1}{3} - \frac{\beta_{11}}{6} - \frac{4}{3} - \beta_{12} - \frac{\beta_{21}}{2} - 2\beta_{22} \\
C_5 &= \frac{1}{3}\left(\frac{\alpha_1}{40} + \frac{4}{15}\alpha_2 - \frac{1}{8}\beta_{11} - 2\beta_{12} - \frac{1}{2}\beta_{21} - 4\beta_{22}\right) \\
C_6 &= \frac{1}{3}\left(\frac{\alpha_1}{240} + \frac{4}{15}\alpha_2 - \frac{1}{40}\beta_{11} - \frac{4}{5}\beta_{12} - \frac{1}{8}\beta_{21} - 2\beta_{22}\right) \\
C_7 &= \frac{1}{3}\left(\frac{\alpha_1}{1680} + \frac{8}{105}\alpha_2 - \frac{1}{240}\beta_{11} - \frac{4}{15}\beta_{12} - \frac{1}{40}\beta_{21} - \frac{4}{5}\beta_{22}\right) \\
C_8 &= \frac{1}{40320}(\alpha_1 + 256\alpha_2) - \frac{1}{5040}(\beta_{11} + 128\beta_{12}) - \frac{1}{720}(\beta_{21} + 64\beta_{22})
\end{aligned}\right\} \quad 3.4$$

with

$$\begin{array}{lll} \alpha_0 = 1 & \beta_{10} = -\tfrac{3}{8} & \beta_{20} = -\tfrac{1}{24} \\ \alpha_1 = -2 & \beta_{11} = 0 & \beta_{21} = \tfrac{1}{3} \\ \alpha_2 = 1 & \beta_{12} = \tfrac{3}{8} & \beta_{22} = -\tfrac{1}{24} \end{array}$$

Substituting these values into equation (3.4) we have

$$C_0 = 1 - 2 + 1 = 0$$

$$C_1 = -2 + 2 + \frac{3}{8} - 0 - \frac{3}{8} = 0$$

$$C_2 = -1 + 2 - 0 - \frac{6}{8} + \frac{1}{24} - \frac{1}{3} + \frac{1}{24} = 0$$

$$C_3 = -\frac{1}{3} + \frac{4}{3} - 0 - \frac{6}{8} - \frac{1}{6} + \frac{1}{12} = 0$$

$$C_4 = -\frac{1}{12} + \frac{2}{3} - 0 - \frac{1}{2} - \frac{1}{6} + \frac{1}{12} = 0$$

$$C_5 = -\frac{1}{20} + \frac{4}{5} - 0 - \frac{3}{3} - \frac{1}{6} + \frac{1}{6} = 0$$

$$C_6 = -\frac{1}{120} + \frac{4}{15} - 0 - \frac{3}{10} - \frac{1}{24} + \frac{1}{12} = 0$$

$$C_7 = -\frac{1}{840} + \frac{8}{105} - 0 - \frac{3}{10} - \frac{1}{120} + \frac{1}{40} = 0$$

$$C_8 = -\frac{1}{6720} + \frac{2}{105} - 0 - \frac{3}{105} - \frac{1}{720} + \frac{1}{90} = 0.0017 \neq 0$$

Implying that $C_0 = C_1 = C_2 = C_3 = C_4 = C_5 = C_6 = C_7 = 0$ and $C_8 = 0.0017$

Hence, method (2.19) is of order 7 with error constant $C_8 = 0.0017$

3.2 Consistency

According to Lambert (1973) and Awoyemi (2001), a linear multi-step method of type (1.4) is consistent if the parameters α_j's and β_{ij}'s satisfy the following conditions:

i. order $P \geq 1$

ii. $\sum_{j=0}^{k} \alpha_j = 0$

iii. $\sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_{ij}$

3.2.1 One-Step First Derivative Method

(i) Since the One-Step First Derivative Method (2.7) is of order 2, then the first condition above is satisfied.

(ii) With $\alpha_0 = -1, \alpha_1 = 1, \beta_{10} = \frac{1}{2}$ and $\beta_{11} = \frac{1}{2}$

$$\sum_{j=0}^{1} \alpha_j = \alpha_0 + \alpha_1$$

$$= -1 + 1$$

$$= 0$$

Also , the second condition is satisfied.

(iii) $\sum_{j=0}^{1} j\alpha_j = 0\alpha_0 + 1\alpha_1$ and $\sum_{j=0}^{1} \beta_{ij} = \beta_{10} + \beta_{11}$

$= 0 + 1$ and $= \frac{1}{2} + \frac{1}{2}$

$= 1$ and $= 1$

Hence, the third condition is satisfied.

Now that all the conditions are satisfied, then the one-step first derivative method is consistent.

3.2.2 One – Step Second Derivative Method

(i) The One – Step Second Derivative method (2.11) is of order 4, then the first condition is satisfied.

(ii) With $\alpha_0 = -1$, $\alpha_1 = 1$, $\beta_{10} = \frac{1}{2}$, $\beta_{11} = \frac{1}{2}$, $\beta_{20} = \frac{1}{12}$ and $\beta_{21} = -\frac{1}{2}$

$$\sum_{j=0}^{1} j\alpha_j = 0\alpha_0 + 1\alpha_1$$

$$= -1 + 1$$

$$= 0$$

Also the second condition is satisfied

(iii) $\sum_{j=0}^{1} j\alpha_j = 0\alpha_0 + 1\alpha_1$ and $\sum_{j=0}^{1} \beta_{ij} = \beta_{10} + \beta_{11} + \beta_{20} + \beta_{21}$

$= 0 + 1$ and $= \frac{-1}{2} + \frac{1}{2} + \frac{1}{12} - \frac{1}{12}$

$= 1$ and $= 1$

meaning that the third condition is satisfied.

Now that all the conditions are satisfied, then the one-step second derivative method is consistent.

3.2.3 Two – Step First Derivative Method

(i)The Two – step second derivative method (2.16) is of order 4, then the first condition is satisfied.

(ii) With, $\alpha_0 = -1$, $\alpha_1 = 0$, $\alpha_2 = 1$, $\beta_{10} = \frac{1}{3}$, $\beta_{11} = \frac{4}{3}$ and $\beta_{12} = \frac{1}{3}$

$$\sum_{j=0}^{2}\alpha_j = \alpha_0 + \alpha_1 + \alpha_2$$

$$= -1 + 0 + 1$$

$$= 0$$

Also, the second condition is satisfied.

(iii) $\sum_{j=0}^{2} j\alpha_j = 0\alpha_0 + 1\alpha_1 + 2\alpha_2$ and $\sum_{j=0}^{2}\beta_{ij} = \beta_{10} + \beta_{11} + \beta_{12}$

$= 0 + 0 + 2$ and $= \frac{1}{3} + \frac{4}{3} + \frac{1}{3}$

$= 2$ and $= 2$

meaning that the third condition is satisfied.

Now that all the conditions are satisfied, then the two-step first derivative method is consistent.

3.2.4 Two – Step Second Derivative Method

(i) The two-step second derivative method (2.19) is of order 7, then the first condition is satisfied.

(ii) With $\alpha_0 = 1$, $\beta_{10} = -\frac{3}{8}$, $\beta_{20} = -\frac{1}{24}$

$\alpha_1 = -2$, $\beta_{11} = 0$, $\beta_{21} = \frac{1}{3}$

$\alpha_2 = 1$, $\beta_{12} = \frac{3}{8}$, $\beta_{22} = -\frac{7}{24}$

$$\sum_{j=0}^{2}\alpha_j = \alpha_0 + \alpha_1 + \alpha_2$$

$$= 1 - 2 + 1$$

$$= 0$$

Also, the second condition is satisfied

(iii) $\sum_{j=0}^{2} j\alpha_j = 0\alpha_0 + 1\alpha_1 + 2\alpha_2$ and $\sum_{j=0}^{2} \beta_{ij} = \beta_{10} + \beta_{11} + \beta_{12} + \beta_{20} + \beta_{21} + \beta_{22}$

$= 0 - 2 + 2$ and $= -\frac{3}{8} + 0 + \frac{3}{8} - \frac{1}{24} + \frac{1}{3} - \frac{7}{24}$

$= 0$ and $= 0$

meaning that the third condition is satisfied.

Now that all the conditions are satisfied, then the two-step second derivative method is consistent.

3.3 Zero – Stability

According to Auzinger *et.al* (1992), Babatola and Ademiluyi, (2007), a linear multistep method of the form:

$$y_{n+k} = \alpha_0 y_n + h\left(\beta_k y'_{n+k} + \beta_0 y'_n\right)$$

with first characteristic polynomial

$$\rho(r) = r^{n+k} - \alpha_0 r^n$$

is said to be zero-stable if the root of the first characteristic polynomial ρ(r) has modulus less than or equal to 1.

This property is checked for all the methods here.

3.3.1 One- Step First Derivative Method

The one – step first derivative method.

$$y_{n+1} = y_n + \frac{h}{2}\left(y'_{n+1} + y'_n\right)$$

whose first characteristic polynomial is

$$\begin{aligned} \rho(r) &= r^{n+1} - r^n = 0 \\ &\quad r^n(r-1) = 0 \end{aligned}$$

and its roots are $r = 0$ or $r = 1$

Showing that the roots are within a unit circle, hence it is zero – stable.

3.3.2 One – Step Second Derivative Method

The one – step second derivative method

$$y_{n+1} = y_n + \frac{h}{2}\left(y'_{n+1} + y'_n\right) - \frac{h^2}{12}\left(y''_{n+1} - y''_n\right)$$

with first characteristic polynomial is

$$\begin{aligned} \rho(r) &= r^{n+1} - r^n = 0 \\ &\quad r^n(r-1) = 0 \end{aligned}$$

Solving we have $r = 0$ or $r = 1$

Since the roots are within a unit circle, the method is zero-stable.

3.3.3 Two- Step First Derivative Method

The Two – Step first Derivative Method

$$y_{n+2} = y_n + \frac{h}{3}\left[y'_{n+2} + 4y'_{n+1} + y'_n\right]$$

whose first characteristic polynomial

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

$$= r^n(r^2 - 1) = 0$$

Solving gives $r = 0$, $r = 1$ or $r = -1$

Since the roots are within a unit circle, the method is zero-stable.

3.3.4 Two Step Second Derivative Method

The Two Step Second Derivative Method

$$y_{n+2} = 2y_{n+1} - y_n + \frac{3}{8}h\left(y'_{n+2} - y'_n\right) + \frac{h^2}{24}\left(y''_{n+2} + 8y'_{n+1} + 8y''_n\right)$$

whose first characteristic polynomial

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

$$r^n\left(r^2 - 2r + 1\right) = 0$$

$$r^n(r-1)^2 = 0$$

Solving gives $r = 0$ or $r = 1$(twice)

Since the roots are within a unit circle, the method is zero-stable.

3.4 Convergence

According to Palencia (1994) and Awoyemi (2005), a necessary and sufficient condition for a linear multistep method to be convergent is that, it must be consistent and zero-stable. From the analysis above, the methods are consistent and zero stable, hence the methods are convergent.

3.5 Absolute Stability of the Methods

A linear multi-step method is said to be absolutely – stable if the region of its stability covers the whole left half of the complex plain.

To ascertain the region of A – stability of the methods, boundary locus method and Dalhquist Stability model test equation ($y' = \lambda y$) are adopted.

3.5.1 One – step first derivative method

Applying the one – step second derivative method

$$y_{n+1} = y_n + \frac{h}{2}\left(y'_{n+1} + y'_n\right)$$

to solve the test equation gives

$$y_{n+1} = y_n + \frac{h}{2}\left(\lambda y_{n+1} + \lambda y_n\right)$$

$$\left(1 - \frac{\lambda h}{2}\right)y_{n+1} = \left(1 + \frac{\lambda h}{2}\right)y_n$$

$$\frac{y_{n+1}}{y_n} = \frac{1 + {\lambda h}/{2}}{1 - {\lambda h}/{2}}$$

Setting $Z = \lambda h$ we obtain

$$\frac{y_{n+1}}{y_n} = \frac{1 + {z}/{2}}{1 - {z}/{2}}$$

where $u(z)$ is called the stability function. This method will produce a convergent approximate if $|u(z)| < 1$

i.e. $\left|\frac{1 + {z}/{2}}{1 - {z}/{2}}\right| < 1$

$$-1 < \frac{1 + {z}/{2}}{1 - {z}/{2}} < 1$$

Simplifying, we have sets A and B with

$$\mathrm{A} = \{z / z < 2\} \text{ and } \quad B = \{z / z < 0\}$$

The region of A – stability is the intersection of sets A and B as shown in the doubly shaded portion of the region in Figure 3.1.

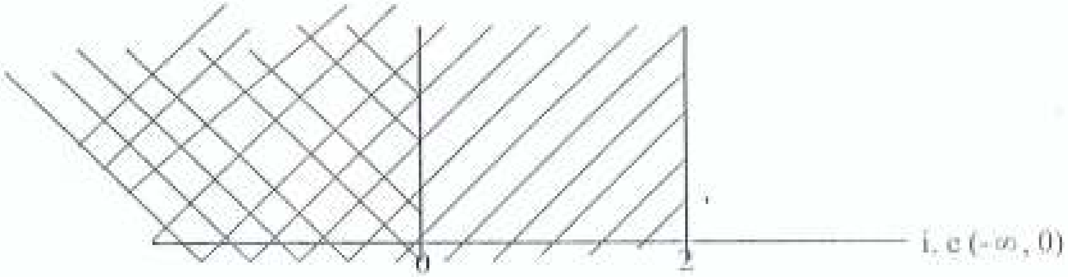


Figure 3.1: Region of Absolute Stability of One-Step First Derivative Method

Hence, the method is A – stable.

3.5.2 One – Step Second Derivative Method

Applying the one – step second derivative method

$$y_{n+1} = y_n + \frac{h}{2}\left(y'_{n+1} + y'_n\right) - \frac{h^2}{12}\left(y''_{n+1} + y''_n\right)$$

to solve the test equation gives

$$y_{n+1} = y_n + \frac{h}{2}\left(\lambda y_{n+1} + \lambda y_n\right) - \frac{h^2}{12}\left(\lambda^2 y_{n+1} + \lambda^2 y_n\right)$$

Simplifying to obtain $z < 2$ or $z < 0$.

The region of A – stability is shown by the doubly shaded portion of the region in Figure 3.2.

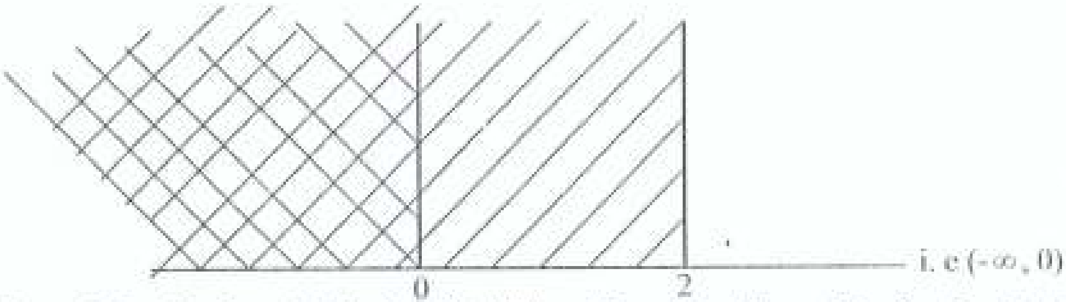


Figure 3.2: Region of Absolute Stability of One-Step Second Derivative Method

Hence the method is A – stable.

3.5.3 Two – step second derivative method

The two – step first derivative method

$$y_{n+2} = y_n + \frac{h}{3}\left[y'_{n+2} + 4y'_{n+1} + y'_n\right]$$

with first characteristic polynomial

$$\rho(r) = r^2 - 1$$

and second characteristic polynomial

$$\delta(r) = \frac{1}{3}\left(r^2 + 4r + 1\right)$$

Applying the boundary locus method; implying

$$h(r) = \frac{\rho(r)}{\delta(r)} \text{ where } r = e^{i\theta} = Cos\theta + i\sin\theta$$

$$h(r) = \frac{r^2 - 1}{\frac{1}{3}\left(r^2 + 4r + 1\right)}$$

$$h(\theta) = \frac{Cos2\theta + i\sin 2\theta - 1}{\frac{1}{3}\left(Cos2\theta + i\sin 2\theta + 4\left(Cos\theta + i\sin\theta\right) + 1\right)}$$

Rationalizing, simplifying and considering only the real part of

$$h(\theta) = x(\theta) + iy(\theta), \quad 0^0 \le \theta \le 180^0$$

gives $x(\theta) = (0,0)$

Hence the method has zero stability only, therefore it is not A – stable.

3.5.4 Two – Step Second Derivative Method

The two – step second derivative method

$$y_{n+2} = 2y_{n+1} - y_n + \frac{3}{8}h\left(y'_{n+2} - y'_n\right) + \frac{h^2}{24}\left(y''_{n+2} + 8y''_{n+1} + 8y''_n\right)$$

with first characteristic polynomial

$\rho(r) = r^2 - 2r + 1$

and second characteristic polynomial

$$\delta(r) = \frac{3}{8}\left(r^2 - 1\right)$$

$$h(r) = \frac{\rho(r)}{\delta(r)} \text{ where } r = e^{i\theta} = Cos\theta + i\sin\theta$$

$$h(\theta) = \frac{8(Cos\theta + i\sin - 1)}{3(Cos\theta + i\sin\theta + 1)}$$

Rationalizing, simplifying and considering only the real part of

$$h(\theta) = x(\theta) + iy(\theta), \quad 0^0 \le \theta \le 180^0$$

gives $x(\theta) = (-\infty, 0)$

The region of A – stability is shown by the doubly shaded portion of the region in Figure 3.3.

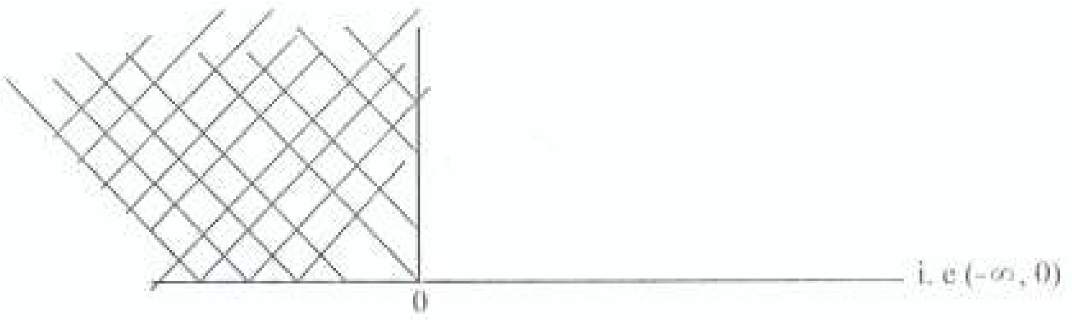


Figure 3.3: Region of Absolute Stability of Two-Step Second Derivative Method

Hence the method is A – stable.

Table 3.1: Summary of the Basic Properties of the Derived Methods

Methods	Error constant	Consistency	Convergence	Interval of A – stability
One – step first derivative *(k = 1, l = 1)*	-0.5	Yes	Yes	$(-\infty, 0)$
One – step second derivative *(k = 1, l = 2)*	0.001389	Yes	Yes	$(-\infty, 0)$
Two – step first derivative *(k = 2, l = 1)*	0.011111	Yes	Yes	$(0, 0)$
Two – step second derivative *(k = 2, l = 2)*	0.000165	Yes	Yes	$(-\infty, 0)$

CHAPTER FOUR

IMPLEMENTATION OF THE METHODS

4.1 Test Problems

To test the suitability and performance of the schemes, the formulae are translated into computer algorithms using FORTRAN programming language. The flow charts are as shown in Figures 4.1 - 4.4. These FORTRAN programmes are used to solve three first order initial value problems of (non-stiff and stiff) ODEs. The results are presented in Tables 4.1 – 4.3. These results are compared with the results of some standard methods like Adams Moulton"s and Addison"s methods as shown in Tables 4.4 – 4.9.

The main aim is to determine the accuracy of the new methods as the order of the derivative and step number are increasing. Because the method is implicit, we require a predictor, that is, a method which is self -starting . It is otherwise called a helper method (Lambert, 1973). The starting methods are predicted by adopting the Taylors series expansion.

Problem 1

A non – stiff I. V. P.

$y' = x + y, \quad y(0) = 1, \quad x \in [0,1]$ with $h = 0.1$

Exact solution: $y(x) = 2e^{x} - x - 1$

Problem 2

A stiff I. V. P.

$y' = -10\left(y - x^3\right) + 3x^2$, $y(0) = 1$ with $h = 0.1$

Exact solution: $y(x) = x^3 + e^{-10x}$

Problem 3

A stiff I. V. P.

$y' = -15y(x)$, $y(0) = 1$ with $h = 0.1$

Exact solution: $y(x) = e^{-15x}$

The results are shown in Tables 4.1 – 4. 4.

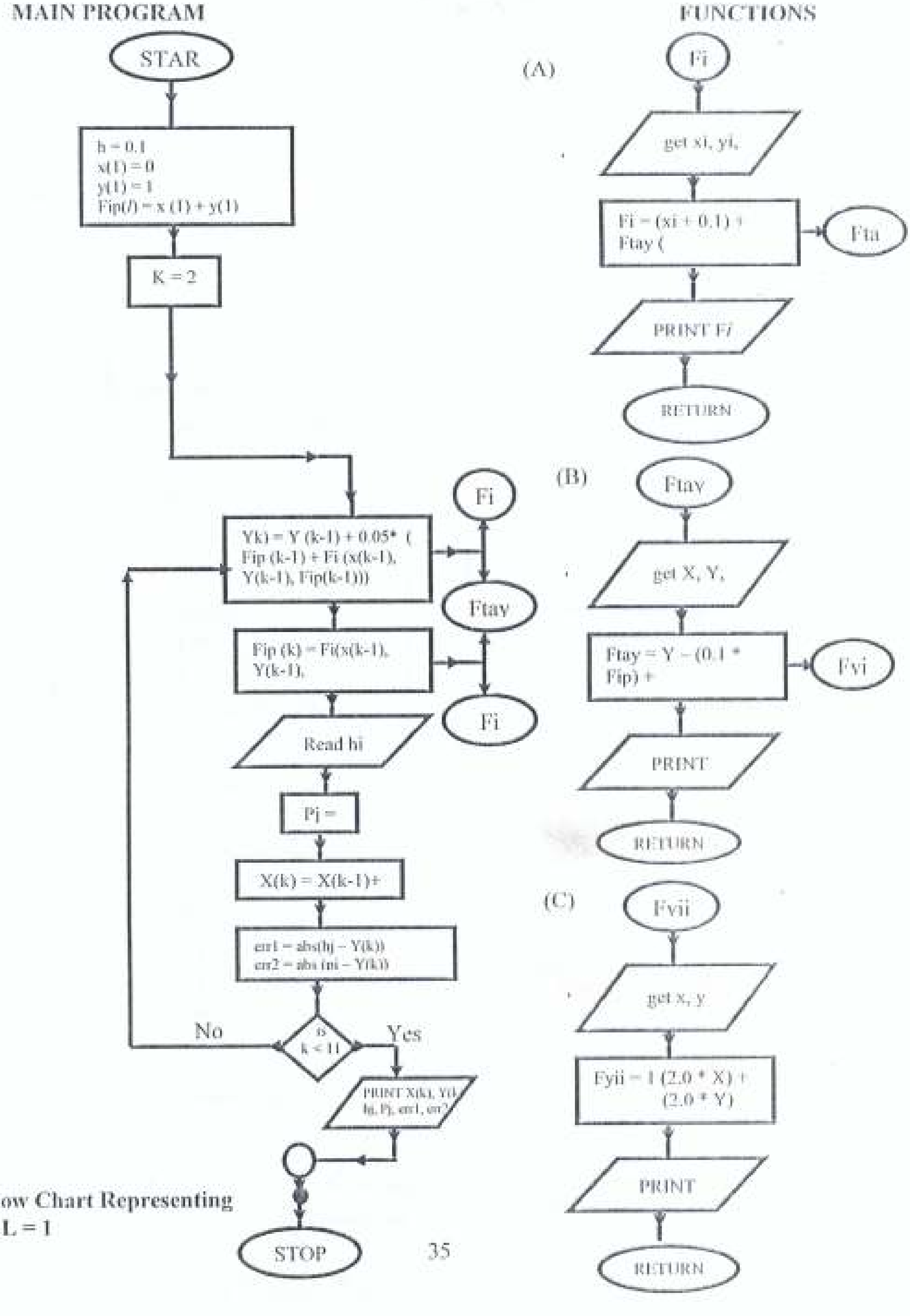
Problem 4

Anon-Linear I.V.

$y' = xy^3 - y$, $y(0) = 1$, $x \in [0,1]$ with $h = 0.1$

Exact solution $y(x) = \dfrac{1}{\sqrt{x + \frac{1}{2}e^{2x}}}$

4.2 The Flow Charts



4.1: Flow Chart Representing
k = 1, L = 1

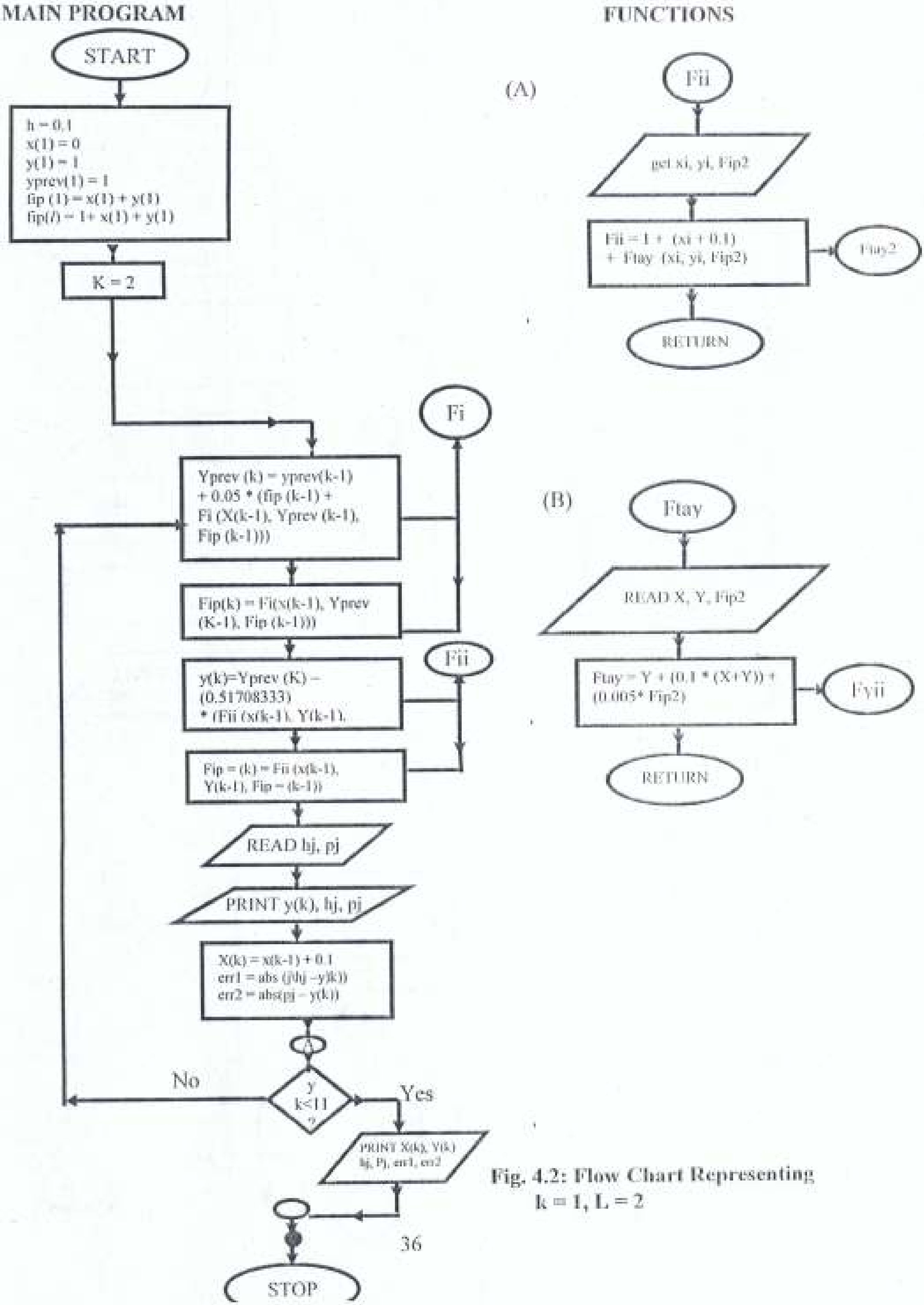


Fig. 4.2: Flow Chart Representing k = 1, L = 2

MAIN PROGRAM

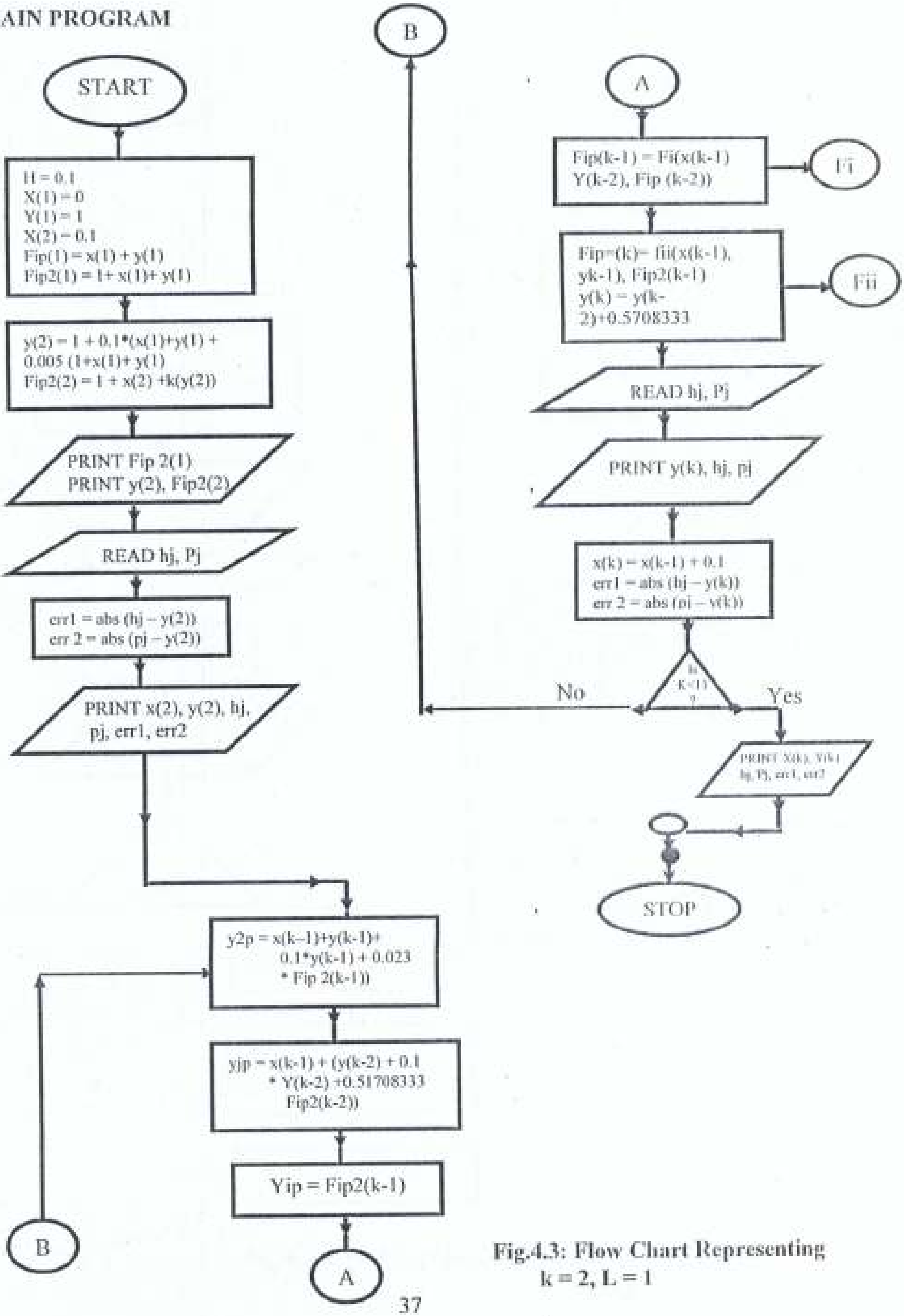


Fig.4.3: Flow Chart Representing
k = 2, L = 1

MAIN PROGRAM

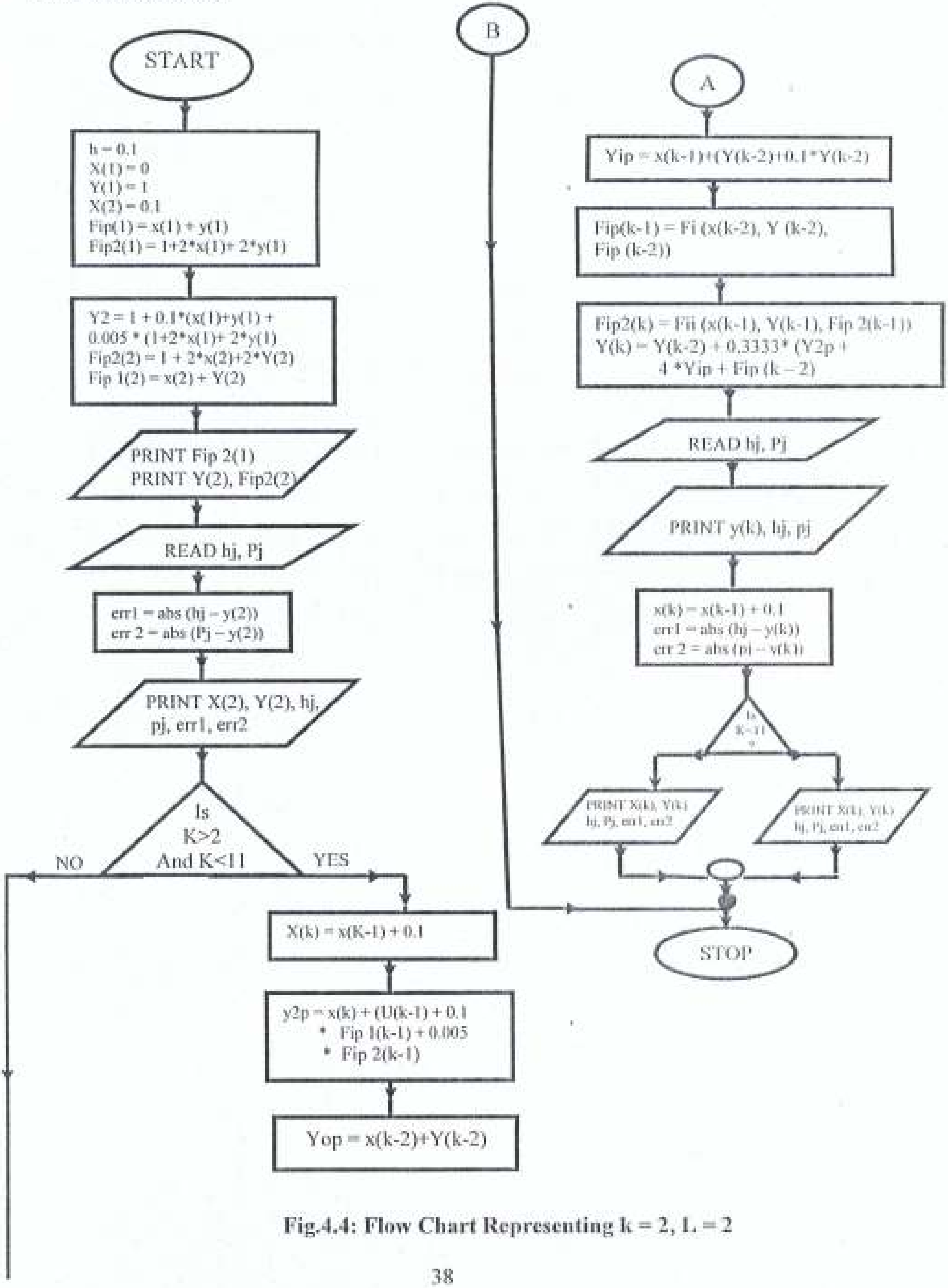


Fig.4.4: Flow Chart Representing k = 2, L = 2

4.3 Tables of Results

Table 4.1: Results Obtained for Problem 1 in Respect of Methods 1-4

Xn	Exact Solution	One Step First Derivative	One step Second Derivative	Two step First Derivative	Two step Second Derivative
0.0	1	1	1	1	1
0.1	1.11034200	1.110000000	1.110341667	1.110341667	1.110341836
0.2	1.24280500	1.242749763	1.242805142	1.242805142	1.242805117
0.3	1.39971800	1.398465250	1.399716994	1.399716994	1.399717616
0.4	1.58364900	1.581804101	1.583648480	1.583648480	1.583649096
0.5	1.79744300	1.794893532	1.797441277	1.797441277	1.797442543
0.6	2.04423800	2.040857353	2.044235924	2.044235924	2.044237602
0.7	2.32750500	2.323147375	2.327503253	2.327503253	2.327505016
0.8	2.65108200	2.645577849	2.651079126	2.651079126	2.651081858
0.9	3.01920600	3.012363523	3.019202827	3.019202827	3.019206023
1.0	3.43656400	3.428161693	3.436559480	3.436559480	3.436563657

Table 4.2: Results Obtained for Problem 2 in Respect of Methods 1-4

Xn	Exact Solution	One Step First Derivative	One step Second Derivative	Two step First Derivative	Two step Second Derivative
0.0	1	1	1	1	1
0.1	0.36788044	0.38150632	0.36842207	0.36840322	0.36788134
0.2	0.60653078	0.60832461	0.60655749	0.60654910	0.60653136
0.3	0.77800800	0.77961324	0.77809183	0.77809099	0.77801042
0.4	0.88249690	0.885632246	0.88258694	0.88256863	0.88249923
0.5	0.93941306	0.94432639	0.93943306	0.93940826	0.93941882
0.6	0.96923323	0.97036215	0.96928343	0.96924644	0.96923723
0.7	0.98449644	0.98540632	0.98449995	0.98445961	0.98449984
0.8	0.99221794	0.99401241	0.99227784	0.99223084	0.99222065
0.9	0.99610137	0.99801243	0.99696487	0.99660078	0.99610605
1.0	0.99804878	0.99967201	0.99808842	0.99802022	0.99804977

Table 4.3: Results Obtained for Problem 3 in Respect of Methods 1-4

Exact Solution	One Step First Derivative	One step Second Derivative	Two step First Derivative	Two step Second Derivative
1	1	1	1	1
3.059023205D-08	3.059611237D-08	3.059062114D-08	3.059062066D-08	3.059023211D-08
6.118046410D-08	6.119936216D-08	6.118050163D-08	6.118050073D-08	6.118046493D-08
9.177069615D-08	9.179463292D-08	9.177096391D-08	9.177096122D-08	9.177069662D-08
1.223609282D-07	1.227323625D-07	1.223613532D-07	1.223613211D-07	1.223609312D-07
1.529511603D-07	1.534632604D-07	1.529520391D-07	1.529520113D-07	1.529511682D-07
1.835413923D-07	1.838360172D-07	1.835463520D-07	1.835463208D-07	1.835413984D-07
2.141316244D-07	2.148069141D-07	2.141324635D-07	2.141324341D-07	2.141316327D-07
2.447218564D-07	2.449721306D-07	2.447301651D-07	2.447301372D-07	2.447218587D-07
2.753129885D-07	2.758314022D-07	2.753243114D-07	2.753243049D-07	2.753129916D-07
3.059023205D-07	3.064125662D-07	3.059042916D-07	3.059042563D-07	3.059023246D-07

Table 4.4: Results Obtained for Problem 4 in Respect of Methods 1-4

Xn	Exact Solution	One Step First Derivative	One step Second Derivative	Two step First Derivative	Two step Second Derivative
0.1	1.18619591	1.17342860	1.18608991	1.48609946	1.48619546
0.2	1.02819279	1.02321363	1.02808143	1.02808285	1.02819223
0.3	0.90869320	0.89461242	0.90856202	0.90856326	0.90869251
0.4	0.81304294	0.80732946	0.81303397	0.81303572	0.81304238
0.5	0.73340497	0.71834675	0.73324162	0.73324329	0.73340436
0.6	0.66518150	0.63103711	0.66501098	0.66501282	0.66518114
0.7	0.60549394	0.58343291	0.60536149	0.60536216	0.60549341
0.8	0.55245110	0.53621495	0.55229052	0.55229196	0.55245094
0.9	0.50476580	0.47365129	0.50459061	0.50459241	0.50476484
1.0	0.46153435	0.43659024	0.46142011	0.46142203	0.46153392

Table 4.5: Comparison of the Second Derivative Methods with Some Existing Methods of the Same Order of Accuracy for Problem One

Xn	Exact Solution	4th Order methods		7th Order methods	
		One step 2nd Derivative	Adams Moulton's method	Two step 2nd Derivative	Addison's method
0.0	1	1	1	1	1
0.1	1.11034200	1.110341667	1.1103413	1.110341667	1.11034167
0.2	1.24280500	1.242805142	1.2428053	1.242805142	1.24280513
0.3	1.39971800	1.399716994	1.3997109	1.399716994	1.39971759
0.4	1.58364900	1.583648480	1.5836480	1.583648480	1.58364948
0.5	1.79744300	1.797441277	1.7974409	1.797441277	1.79744228
0.6	2.04423800	2.044235924	2.0442347	2.044235924	2.04423697
0.7	2.32750500	2.327503253	2.3275032	2.327503253	2.32750506
0.8	2.65108200	2.651079126	2.6510787	2.651079126	2.65108173
0.9	3.01920600	3.019202827	3.0192016	3.019202827	3.01920604
1.0	3.43656400	3.436559480	3.4365579	3.436559480	3.43656249

Table 4.6; Comparison of the Second Derivative Methods with Some Existing Methods of the Same Order of Accuracy for Problem Two

Xn	Exact Solution	4th Order methods		7th Order methods	
		One step 2nd Derivative	Adams Moulton's method	Two step 2nd Derivative	Addison's method
0.0	1	1	1	1	1
0.1	0.36788044	0.36842207	0.37500103	0.36788134	0.36789134
0.2	0.60653078	0.60655749	0.60677096	0.60653136	0.60653872
0.3	0.77800800	0.77809183	0.77880861	0.77801042	0.77801882
0.4	0.88249690	0.88258694	0.88279715	0.88249923	0.88250148
0.5	0.93941306	0.93943306	0.93951307	0.93941882	0.93941936
0.6	0.96923323	0.96928343	0.96943323	0.96923723	0.96923899
0.7	0.98449644	0.98449995	0.98519644	0.98449984	0.98450280
0.8	0.99221794	0.99227784	0.99231794	0.99222065	0.99222247
0.9	0.99610137	0.99696487	0.99730137	0.99610605	0.99610729
1.0	0.99804878	0.99808842	0.99824878	0.99804977	0.99806346

Table 4.7: Comparison of the Second Derivative Methods with Some Existing Methods of the Same Order of Accuracy for Problem Three

Xn	Exact Solution	4th Order methods		7th Order methods	
		One step 2nd Derivative	Adams Moulton's method	Two step 2nd Derivative	Addison's method
0.1	3.059023205D-08	3.059062114D-08	3.059063126D-08	3.059023211D-08	3.059023229D-08
0.2	6.118046410D-08	6.118050163D-08	6.118050621D-08	6.118046493D-08	6.118046533D-08
0.3	9.177069615D-08	9.177096391D-08	9.177098103D-08	9.177069662D-08	9.177069892D-08
0.4	1.223609282D-07	1.223613532D-07	1.223613742D-07	1.223609312D-07	1.223609543D-07
0.5	1.529511603D-07	1.529520391D-07	1.529528016D-07	1.529511682D-07	1.529511827D-07
0.6	1.835413923D-07	1.835463520D-07	1.835465331D-07	1.835413984D-07	1.835414036D-07
0.7	2.141316244D-07	2.141324635D-07	2.141326461D-07	2.141316327D-07	2.141316541D-07
0.8	2.447218564D-07	2.447301651D-07	2.447321143D-07	2.447218587D-07	2.447218729D-07
0.9	2.753129885D-07	2.753243114D-07	2.753245367D-07	2.753129916D-07	2.753130052D-07
1.0	3.059023205D-07	3.059042916D-07	3.059043972D-07	3.059023246D-07	3.059023429D-07

Table 4.8: Comparison of the Second Derivative Methods with Some Existing Methods of the Same Order of Accuracy for Problem Four

Xn	Exact Solution	4th Order methods		7th Order methods	
		One step 2nd Derivative	Adams Moulton's method	Two step 2nd Derivative	Addison's method
0.1	1.18619591	1.18608991	1.18432106	1.18619546	1.18619215
0.2	1.02819279	1.02808143	1.02631423	1.02819223	1.02818996
0.3	0.90869320	0.90856202	0.90611348	0.90869251	0.90868878
0.4	0.81304294	0.81303397	0.81096433	0.81304238	0.81304062
0.5	0.73340497	0.73324162	0.73193761	0.73340436	0.73340372
0.6	0.66518150	0.66501098	0.66343672	0.66518114	0.66517891
0.7	0.60549394	0.60536149	0.60241736	0.60549341	0.60549102
0.8	0.55245110	0.55229052	0.55053246	0.55245094	0.55245036
0.9	0.50476580	0.50459061	0.50114363	0.50476484	0.50476092
1.0	0.46153435	0.46142011	0.45983722	0.46153392	0.46153165

Table 4.9: Percentage Errors of the 2nd Derivative Methods and Some Existing Multi-step Methods in Respect of Problem One

Xn	One Step 2nd Derivative method	Adams Moulton's method	Two – step 2nd Derivative	Addison's method
0.1	2.999	6.304	1.477	2.972
0.2	1.143	2.413	0.942	0.942
0.3	7.187	50.724	2.743	2.929
0.4	3.284	6.315	0.610	3.031
0.5	9.586	11.683	2.543	4.006
0.6	8.500	16.143	1.947	5.039
0.7	7.506	7.734	0.688	2.578
0.8	11.218	12.448	10.811	10.928
0.9	10.509	14.573	0.762	9.595
1.0	13.153	17.750	0.998	4.394

Table 4.10: Percentage Errors of The 2nd Derivative Methods and Some Existing Multi-step Methods in Respect of Problem Two

Xn	One Step 2nd Derivative method	Adams Moulton's method	Two – step 2nd Derivative	Addison's method
0.1	1.472	19.356	2.446	29.630
0.2	0.044	0.396	0.956	13.091
0.3	0.108	1.029	3.111	13.907
0.4	0.102	0.340	2.640	5.190
0.5	0.021	0.107	6.166	6.744
0.6	0.052	0.206	4.127	5.943
0.7	0.036	0.711	3.413	6.460
0.8	0.060	0.101	2.731	4.566
0.9	0.851	1.205	4.698	5.943
1.0	0.040	0.200	0.992	1.513

Table 4.11: Percentage Errors of the 2^{nd} Derivative Methods and Some Existing Multi-step Methods in Respect to Problem Three

Xn	One Step 2^{nd} Derivative method	Adams Moulton's method	Two – step 2nd Derivative	Addison's method
0.1	1.272	1.305	0.020	0.078
0.2	0.613	0.688	1.357	1.994
0.3	2.918	3.104	0.512	3.018
0.4	0.347	0.365	0.245	2.133
0.5	0.575	1.073	0.517	1.465
0.6	2.702	2.801	0.332	0.616
0.7	0.392	0.477	0.388	1.387
0.8	34.220	42.249	0.947	6.780
0.9	4.112	4.194	0.113	0.607
1.0	0.644	0.679	0.134	0.732

Table 4.12: Percentage Errors of the 2^{nd} Derivative Methods and Some Existing Multi-step Methods in Respect to Problem Four

Xn	One Step 2^{nd} Derivative method	Adams Moulton's method	Two – step 2nd Derivative	Addison's method
0.1	0.894	15.8	3.80	31.7
0.2	0.127	18.3	5.45	27.5
0.3	0.144	28.4	7.59	48.6
0.4	0.703	25.6	6.89	28.5
0.5	0.304	20.0	8.32	16.1
0.6	0.256	26.2	5.41	38.9
0.7	0.219	50.8	8.75	37.8
0.8	0.291	62.9	2.90	13.3
0.9	0.347	71.7	9.01	96.7
1.0	0.248	36.8	9.32	58.5

4.4: Graphical Illustration of Errors of the Methods

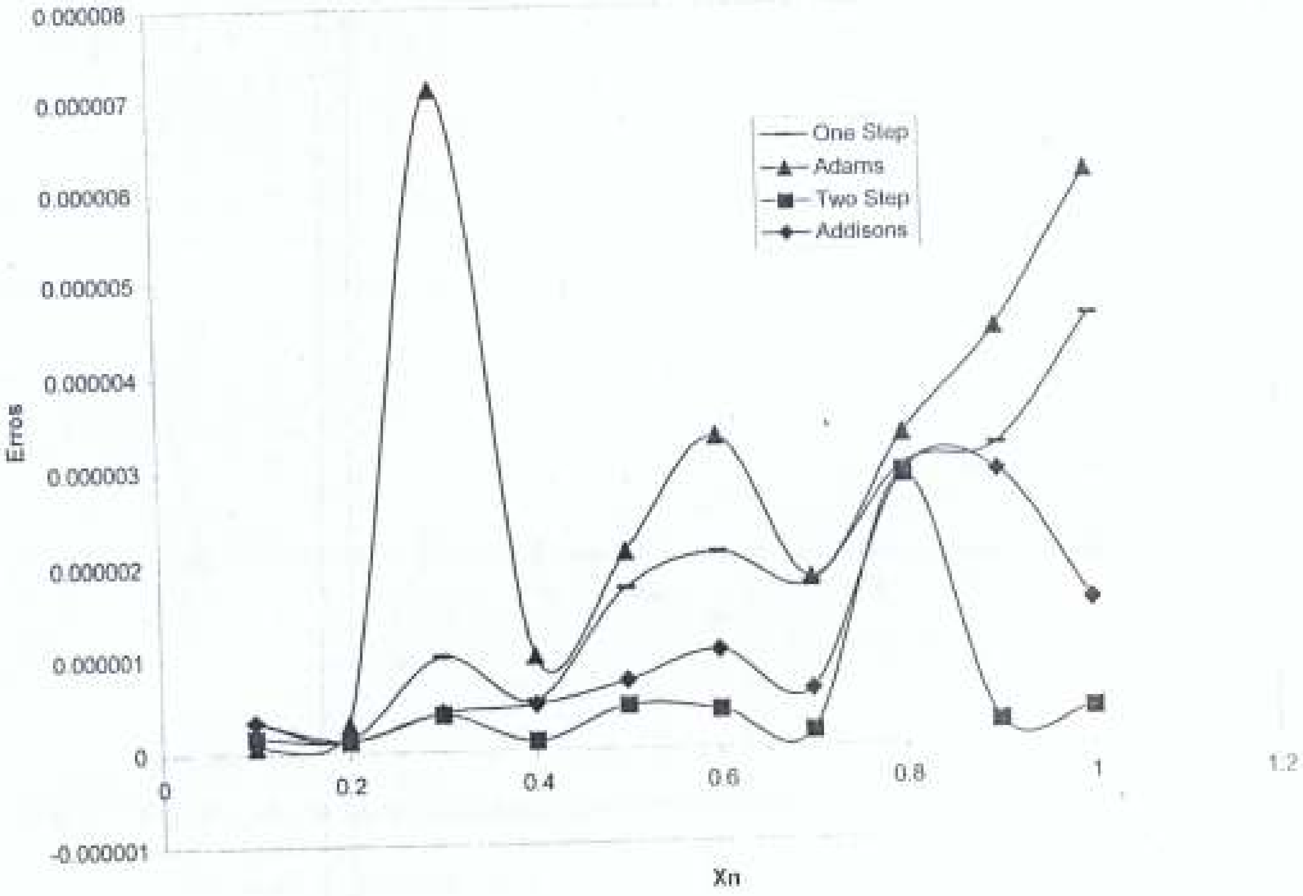


Figure 4.5: Errors of Second Derivative Methods and Some Existing LMM with Respect to Problem one

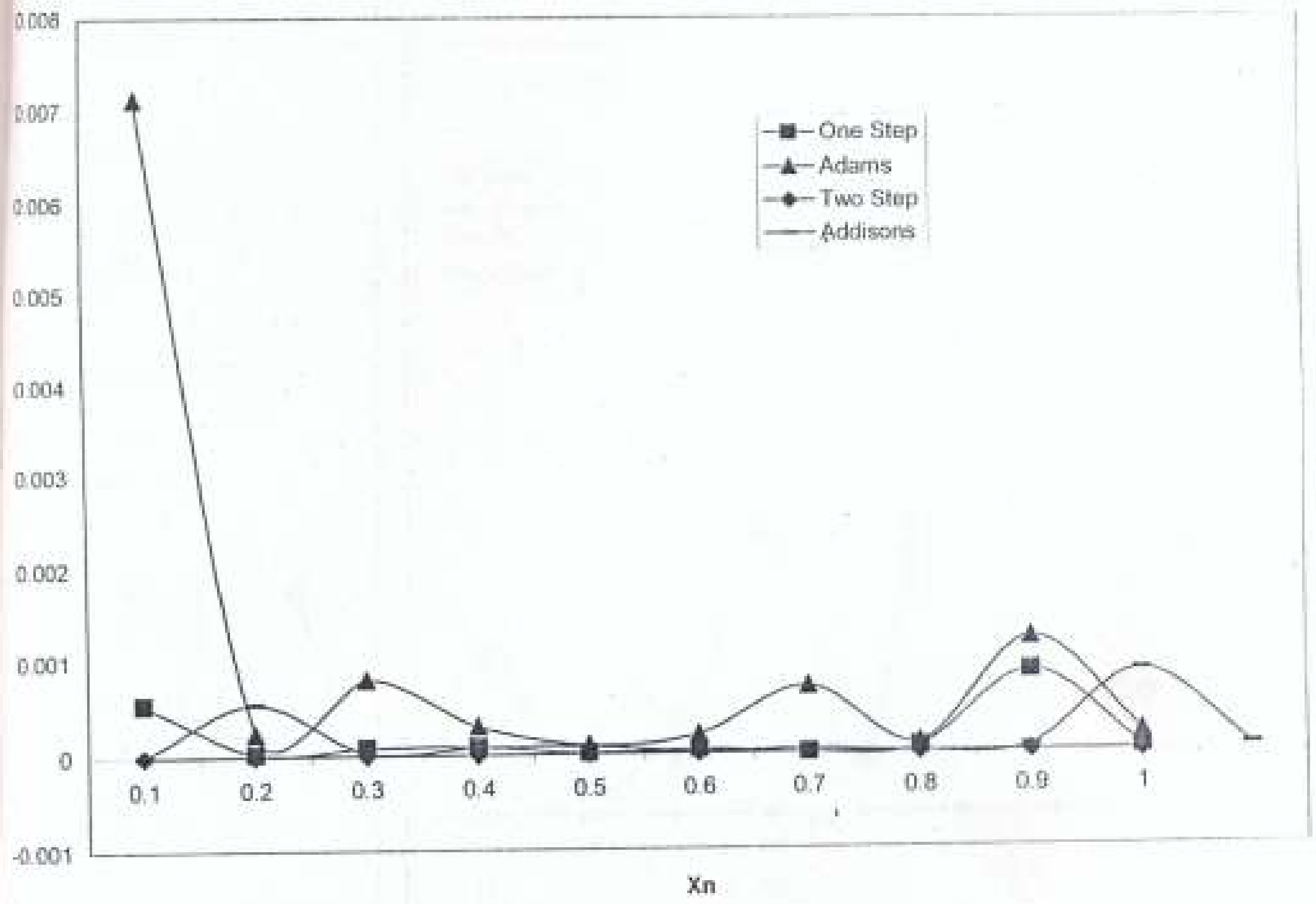


Figure 4.6: Errors of Second Derivative Methods and Some Existing LMM with Respect to Problem Two

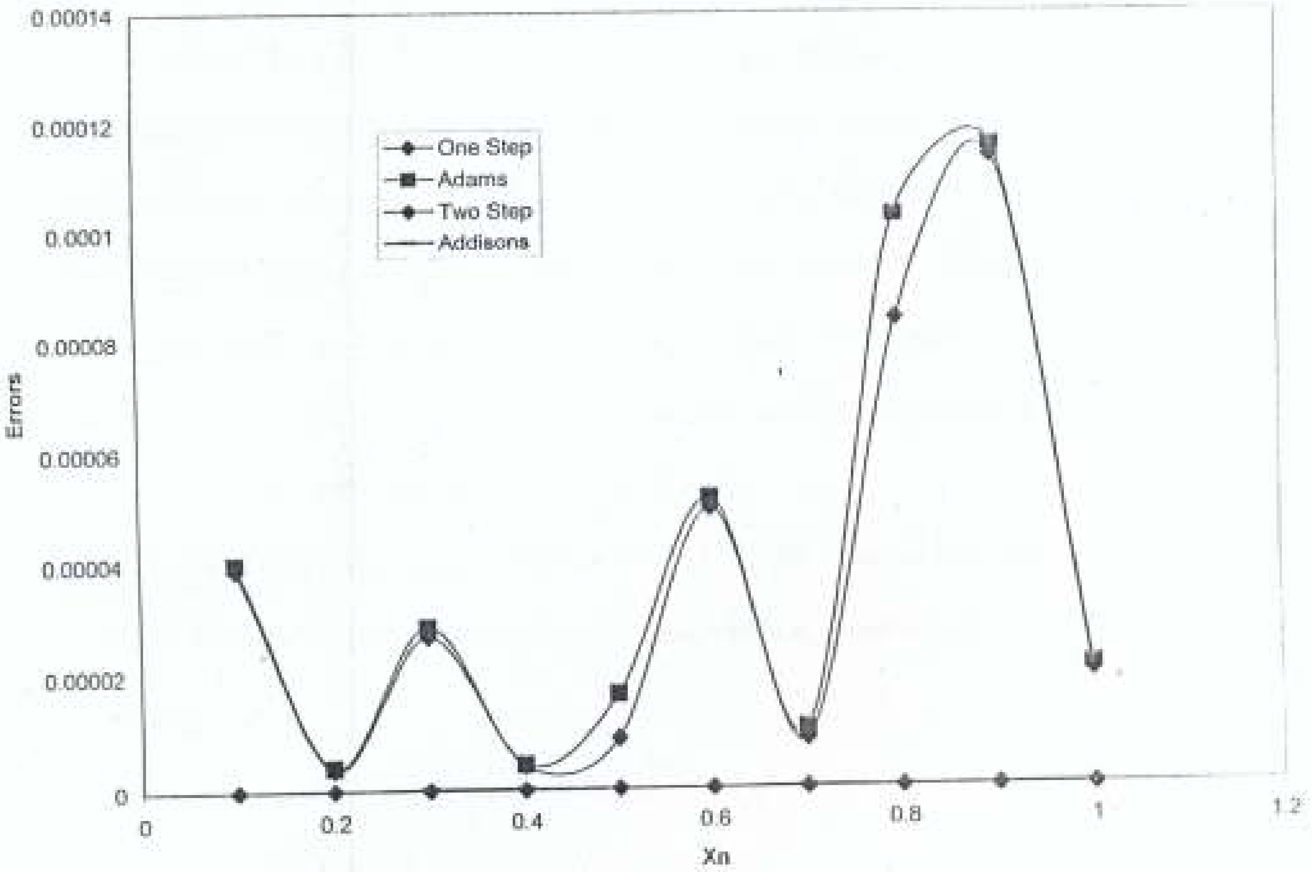


Figure 4.7: Errors of Second Derivative Methods and Some Existing LMM with Respect to Problem Three

4.5 Discussion of Results

Tables 4.1 – 4.4 shows that the accuracy of the methods improves as the order of the derivative increases, that is, the one – step second derivative method has better accuracy when compared with one – step first derivative method. Also, the two – step second derivative method is more accurate than the two – step first derivative.

It can also be observed that as the step – size (k) of the method increases, better accuracy is achieved. Consequently, the two – step methods for which k = 2 are more accurate than the one – step methods for which k = 1.

The Tables of results in Tables 4.5 – 4.12 also showed that the new methods compare favourably with Adam's Moulton and Addison's methods of the same order of accuracy.

CHAPTER FIVE

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusion

In this study, a class of implicit multi-derivative linear multi-step methods have been developed for numerical solution of first order ordinary differential equations. Analysis of the basic properties showed that the methods are consistent, zero – stable, convergent and absolutely stable. Suggesting that the methods are suitable for the solution of non – stiff and stiff Initial Value Problems of Ordinary Differential Equations.

The numerical implementation of the schemes requires the transformation of the schemes to FORTRAN programmes, used to solve some sample initial value problems of first order ODEs. The results are shown in Tables 4.1 – 4.4. It is clear that second derivative methods seem to give better accuracy than first derivative methods.

The results in Tables (4.5 – 4.12) also show that the new schemes compare favourably with Adam's and Addison's Linear Multi-step methods.

5.2 Limitations and Recommendations

In this work, Taylor series was adopted as the basic function, although, other basic functions could be adopted to see whether accuracy will be improved.

It is suggested that higher derivatives should be investigated and adopted when good accuracy is the focus. Also, a step size (h) lower than 0.1 can be used to implement the methods to see whether accuracy will be improved.

Furthermore, the explicit aspect of multi-derivative linear multi-step methods for the solution of first order ordinary differential equations should be studied.

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