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Full Length Research Paper

A comparative study of a class of implicit multi-derivative methods for numerical solution of non-stiff and stiff first order ordinary differential equations

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This work describes the development, analysis, implementation and a comparative study of a class of Implicit Multi-derivative Linear Multistep methods for numerical solution of non-stiff and stiff Initial Value Problems of first order Ordinary Differential Equations. These multi-derivative methods incorporate more analytical properties of the differential equation into the conventional implicit linear multistep formulae and vary the step-size (k) as well as the order of the derivative (l) to obtain more accurate and efficient methods for solution of non-stiff and stiff first order ordinary differential equations. The basic properties of these methods were analyzed and the results showed that the methods are accurate, convergent and A-stable. Hence, suitable for the solution of non-stiff and stiff initial value problems of ordinary differential equations. A comparative study of the newly developed methods are carried out to determine the effect of increasing the step-size (k) and the order of the derivative (l). The result showed a remarkable improvement in accuracy and efficiency as the step-size (k) and the order of the derivative (l) are increased.

Key words: Implicit, Multi-derivative, Multi-step, Non-stiff, Stiff, Ordinary and Differential equation.

INTRODUCTION

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. (Awoyemi, 1992).Consequently, it constitutes a large and very important aspect of today's mathematics. Though, these problems exist by theory or principle, their mathematical analyses give rise to differential equations, because the objects involved obey certain physical and chemical laws involving rates of change (Ross, 1989; Auzinger et al., 1990; Courant, 2007). Only a few of these differential equations can be solved analytically, this reason gave the search for numerical approximation.

Ordinary differential equations (ODEs) can be classified into two: Initial value problem (IVP) or boundary value problem (BPV) depending upon the given condition(s) (Ademiluyi and Kayode, 2000).

A differential equation together with initial condition prescribed at one point is called IVP. For example the differential equation:

$y^1= x+ y, y(0) = 1$

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:

$$y' = f(x,y), y(x_0) = y_0, a \leq x \leq b \tag{1}$$

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

A Linear Multi-step Method (LMM) for numerical solution of first order ordinary differential equations of the kind (1) is a computational method of the form:

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$$\sum_{j=0}^{k} \alpha_j \, y_{n+j} = h \sum_{j=0}^{k} \beta_j \, y'_{n+j} \qquad (2)$$

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; Jain, 1984).

In this study, we consider the development of methods for which k=1 and 2 respectively with the inclusion of more analytical properties of the differential equation by way of more derivative properties of the differential equation. The study also attempts to determine the effect of increasing the order of the derivatives as well as varying the step-size of the Linear Multistep Methods of the form:

$$\sum_{j=0}^{k} \alpha_j \, y_{n+j} \;=\; \sum_{i=1}^{l} h^i \sum_{j=0}^{k} \beta_{ij} \, y^i{}_{n+j}; \;\; \alpha_k = +1 \qquad (3)$$

which involves more derivative properties of the differential equation. The aim of this study is to compare the accuracy and stability of some implicit multi-derivative linear multi-step methods.

DERIVATION OF THE METHODS

Linear multistep methods of the Form 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, implementation and a comparative study of a family of implicit multiderivative linear multistep methods. That is, methods for which $\beta_k \neq 0$. To achieve this, the local truncation error Formula 5 to determine parameters α_j's and β_{ij}'s of the Formula 4 for step numbers k = 1and 2 was considered. Consequently, it is assumed that the local truncation error T_{n+k} for step application of the formula to problem 1 (Equation 1) can be defined as:

$$T_{n+k} = \sum_{j=0}^{k} \alpha_j \, y_{n+j} \; - \; \sum_{i=1}^{l} h^i \sum_{j=0}^{k} \beta_{ij} \, y^i{}_{n+j} \qquad (4)$$

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:

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

in Equation 4 and combine terms in equal powers of h, we have:

$$T_{n+k} = C_o y_n + C_1 h y'_n + C_2 h^2 y''_n + \ldots C_p h^p y^p + \ldots (h^{P+1}) \qquad (5)$$

where:

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

One – step first derivative method

Setting k = 1, l = 1 in Equation 4 gives:

$$\alpha_0 y_n + \alpha_1 y_{n+1} = h\beta_{10} y'_n + h\beta_{11} y'_{n+1} \qquad (6)$$

with local truncation error:

$$T_{n+1} = \alpha_0 y_n + \alpha_1 y_{n+1} - h\beta_{10} y'_n - h\beta_{11} y'_{n+1} \qquad (7)$$

The Taylor's expansion of:

$$y_{n+1} = y_n + h y'_n + \frac{h^2 y''}{2!} + \frac{h^3 y^{iii}}{3!} + \ldots\ldots + 0(h^4) \qquad (8)$$

and;

$$y'_{n+1} = y'_n + h y^{ii}_n + \frac{h^2 y^{iii}}{2!} + \frac{h^3 y^{ivi}}{3!} + \ldots\ldots + 0(h^4) \qquad (9)$$

Substituting these into Equation 7 and combine terms in equal powers of h, gives:

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

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,

$$\alpha_0 + \alpha_1 = 0$$

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

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

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

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

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

Substituting these values into Equation 6 and simplifying to obtain a one-step first derivative method of the form:

$$y_{n+1} = y_n + \frac{h}{2}\left(y'_{n+1} + y'_n\right) \tag{10}$$

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

One – step second derivative method

Setting $k = 1, l = 2$ in (4) gives:

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

with local truncation error:

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

Adopting the Taylor's series expansion of y_{n+1} and y^1_{n+1} as in Equations 8 and 9 respectively and;

$$y^{ii}_{n+1} = y^{ii}_n + h y^{iii}_n + \frac{h^2 y^{iv}}{2!} + \frac{h^3 y^{vi}}{3!} + \ldots\ldots + 0(h^4) \tag{13}$$

in Equation 12, combining terms in equal powers of h gives:

$$T_{n+1} = C_o y_n + C_1 h y'_n + C_2 h^2 y''_n + C_3 h^3 y^{iii}_n$$

$$+ C_4 h^4 y^{iv}_n + 0\left(h^5\right)$$

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, the following system of linear equations were obtained:

$\alpha_0 + \alpha_1 = 0$

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

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

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

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

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

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 11 and simplifying to obtain a one step linear multi-derivative multistep formula:

$$y_{n+1} = y_n + \frac{h}{2}\left[y'_{n+1} + y'_n\right] - \frac{h^2}{12}\left[y''_{n+1} - y''_n\right] \tag{14}$$

Two – step first derivative linear multi-step method

Setting $k = 2, l = 1$ in (4), gives:

$$\alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} = h\left[\beta_{10} y'_n + \beta_{11} y'_{n+1} + \beta_{12} y'_{n+2}\right] \tag{15}$$

with local truncation error:

$$T_{n+2} = \alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_2 y_{n+2} - h[\beta_{10} y'_n + \beta_{11} y'_{n+1} + \beta_{12} y'_{n+2}] \qquad (16)$$

Adopting the Taylor's series expansion of y_{n+1}, y^1_{n+1}, y_{n+2} and $y^i{}_{n+2}$ as given in Equations 8, 9, 17 and 18 in Equation 16:

$$y_{n+2} = y_n + 2hy^i_n + \frac{4h^2 y^{ii}}{2!} + \frac{8h^3 y^{iii}}{3!} + ...+ 0(h^4) \qquad (17)$$

$$y^i_{n+2} = y^i_n + 2hy^{ii}_n + \frac{4h^2 y^{iii}}{2!} + \frac{8h^3 y^{iv}}{3!} + ...+ 0(h^4) \qquad (18)$$

and combine terms in equal power of h gives:

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

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 α_2=1gives:

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

Substituting these values into Equation 15 and simplifying we obtain a two-step first derivative
formula of the form:

$$y_{n+2} = y_n + \frac{h}{3}\left(y'_{n+2} + 4y'_{n+1} + y'_n\right) \qquad (19)$$

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

Two – step second derivative linear multi-step method

Setting $k=2, l=2$ in (4) gives:

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

with local truncation error:

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

………… (21)

Adopting the Taylor's series expansion of y_{n+1}, y^1_{n+1}, y_{n+2} and y^1_{n+2} as in Equations 8, 9, 17 and 18 in Equation 21 and combine terms in equal powers of h gives:

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

Where;

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

$$C_1 = \alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12}$$
$$C_2 = \frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12} - \beta_{20} - \beta_{21} - \beta_{22}$$
$$C_3 = \frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{12} - \beta_{21} - 2\beta_{22}$$
$$C_4 = \frac{\alpha_1}{24} + \frac{2\alpha_1}{3} - \frac{\beta_{11}}{6} - \frac{4}{3} - \beta_{12} - \frac{\beta_{21}}{2} - 2\beta_{22}$$

$$C_5 = \frac{1}{3}\left(\frac{\alpha_1}{40} + \frac{4}{15}\alpha_2 - \frac{1}{8}\beta_{11} - 2\beta_{12} - \frac{1}{2}\beta_{21} - 4\beta_{22}\right)$$
$$C_6 = \frac{1}{3}\left(\frac{\alpha_1}{240} + \frac{4}{15}\alpha_2 - \frac{1}{40}\beta_{11} - \frac{4}{5}\beta_{12} - \frac{1}{8}\beta_{21} - 2\beta_{22}\right)$$
$$C_7 = \frac{1}{3}\left(\frac{\alpha_1}{1680} + \frac{8}{105}\alpha_2 - \frac{1}{240}\beta_{11} - \frac{4}{15}\beta_{12} - \frac{1}{40}\beta_{21} - \frac{4}{5}\beta_{22}\right)$$
$$C_8 = \frac{1}{40320}(\alpha_1 + 256\alpha_2) - \frac{1}{5040}(\beta_{11} + 128\beta_{12}) - \frac{1}{720}(\beta_{21} + 64\beta_{22})$$

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:

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

Substituting these values into Equation 20 and simplifying we obtain a two-step second derivative formula of the form:

$$y_{n+2} = 2y_{n+1} - y_n + \frac{3h}{8}\left(y'_{n+2} - y'_n\right) - \frac{h^2}{24}\left(y''_{n+2} - 8y''_{n+1} + y''_n\right) \quad (22)$$

Basics properties of the methods

According to Gear (1971), a good numerical method for solution of ordinary differential equations is required to be accurate, consistent, zero-stable, convergent and absolutely-stable, these were investigated.

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; Dahlquist, 1978). 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.

One-step first derivative method

For the One-Step First Derivative Method (10) the local truncation error:

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

where;

$$\left.\begin{array}{l} C_0 = \alpha_0 + \alpha_1 \\ C_1 = \alpha_1 - \beta_{10} - \beta_{11} \\ C_2 = \tfrac{1}{2}\alpha_1 - \beta_{11} \\ C_3 = \tfrac{1}{6}\alpha_1 - \tfrac{1}{2}\beta_{11} \end{array}\right\} \quad (23)$$

with;

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

Substituting these values into Equation 23 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 (10) is of order 2 with error constant $C_3 = -\frac{1}{12}$

One-step second derivative method

For the one-step second derivative method (14) the local truncation error:

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

where;

$$C_0 = \alpha_0 + \alpha_1$$
$$C_1 = \alpha_1 - \beta_{10} - \beta_{11}$$
$$C_2 = \frac{\alpha_1}{2} - \beta_{11} - \beta_{20} - \beta_{21}$$
$$C_3 = \frac{\alpha_1}{6} - \frac{\beta_{11}}{2} - \beta_{21}$$
$$C_4 = \frac{\alpha_1}{24} - \frac{\beta_{11}}{6} - \frac{\beta_{21}}{2}$$
$$C_5 = \frac{\alpha_1}{120} - \frac{\beta_{11}}{24} - \frac{\beta_{21}}{6}$$

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 24 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; $C_0 = C_1 = C_2 = C_3 = C_4 = 0$,

$$C_5 = \frac{1}{720} \quad \neq 0$$

Hence, method (14) is of order 4 with error constant

$$C_5 = \frac{1}{720}$$

Two-step first derivative method

For the two-step first derivative method (19) the local truncation error:

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

where;

$$C_0 = \alpha_0 + \alpha_1 + \alpha_1$$
$$C_1 = \alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12}$$
$$C_2 = \frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12}$$
$$C_3 = \frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{12}$$
$$C_4 = \frac{\alpha_1}{24} + \frac{2}{3}\alpha_2 - \frac{\beta_{11}}{6} - \frac{4}{3}\beta_{12}$$
$$C_5 = \frac{1}{120}\alpha_1 - \frac{4}{15}\alpha_2 + \frac{1}{24}\beta_{11} + \frac{2}{3}\beta_{12}$$

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 25 gives:

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

$$C_1 = 0 - 2 - \frac{1}{3} - \frac{4}{3} - \frac{1}{3} = 0$$
$$C_2 = 0 + 2 - \frac{4}{3} - \frac{2}{3} = 0$$
$$C_3 = 0 + \frac{4}{3} - \frac{4}{6} - \frac{2}{3} = 0$$
$$C_4 = 0 + \frac{2}{3} - \frac{4}{18} - \frac{4}{9} = 0$$
$$C_5 = 0 - \frac{4}{15} - \frac{4}{72} - \frac{2}{9} = \frac{1}{90}$$

Implying that; $C_0 = C_1 = C_2 = C_3 = C_4 = 0$, and

$$C_5 = \frac{1}{90} \neq 0$$

Hence, method (19) is of order 4 with error constant

$$C_5 = \frac{1}{90}$$

Two-step second derivative method

For the two-step second derivative method (22) the local truncation error:

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

where;

$$C_0 = \alpha_0 + \alpha_1 + \alpha_2$$
$$C_1 = \alpha_1 + 2\alpha_2 - \beta_{10} - \beta_{11} - \beta_{12}$$
$$C_2 = \frac{\alpha_1}{2} + 2\alpha_2 - \beta_{11} - 2\beta_{12} - \beta_{20} - \beta_{21} - \beta_{22}$$
$$C_3 = \frac{\alpha_1}{6} + \frac{4}{3}\alpha_2 - \frac{\beta_{11}}{2} - 2\beta_{12} - \beta_{21} - 2\beta_{22}$$
$$C_4 = \frac{\alpha_1}{24} + \frac{2\alpha_1}{3} - \frac{\beta_{11}}{6} - \frac{4}{3} - \beta_{12} - \frac{\beta_{21}}{2} - 2\beta_{22}$$
$$C_5 = \frac{1}{3}\left(\frac{\alpha_1}{40} + \frac{4}{15}\alpha_2 - \frac{1}{8}\beta_{11} - 2\beta_{12} - \frac{1}{2}\beta_{21} - 4\beta_{22}\right)$$
$$C_6 = \frac{1}{3}\left(\frac{\alpha_1}{240} + \frac{4}{15}\alpha_2 - \frac{1}{40}\beta_{11} - \frac{4}{5}\beta_{12} - \frac{1}{8}\beta_{21} - 2\beta_{22}\right)$$

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

with;

$$\alpha_0 = 1 \quad \beta_{10} = -3/8 \quad \beta_{20} = -1/24$$
$$\alpha_1 = -2 \quad \beta_{11} = 0 \quad \beta_{21} = 1/3$$
$$\alpha_2 = 1 \quad \beta_{12} = 3/8 \quad \beta_{22} = -1/24$$

Substituting these values into Equation 27 gives:

$$C_0 = 1 - 2 + 1 = 0$$
$$C_1 = -2 + 2 + \frac{3}{8} - 0 - \frac{3}{8} = 0$$
$$C_2 = -1 + 2 - 0 - \frac{6}{8} + \frac{1}{24} - \frac{1}{3} + \frac{1}{24} = 0$$
$$C_3 = -\frac{1}{3} + \frac{4}{3} - 0 - \frac{6}{8} - \frac{1}{6} + \frac{1}{12} = 0$$
$$C_4 = -\frac{1}{12} + \frac{2}{3} - 0 - \frac{1}{2} - \frac{1}{6} + \frac{1}{12} = 0$$
$$C_5 = -\frac{1}{20} + \frac{4}{5} - 0 - \frac{3}{3} - \frac{1}{6} + \frac{1}{6} = 0$$
$$C_6 = -\frac{1}{120} + \frac{4}{15} - 0 - \frac{3}{10} - \frac{1}{24} + \frac{1}{12} = 0$$
$$C_7 = -\frac{1}{840} + \frac{8}{105} - 0 - \frac{3}{10} - \frac{1}{120} + \frac{1}{40} = 0$$
$$C_8 = -\frac{1}{6720} + \frac{2}{105} - 0 - \frac{3}{105} - \frac{1}{720} + \frac{1}{90} = 0.0017 \neq 0$$

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 (22) is of order 7 with error constant

$$C_8 = 0.0017$$

Consistency

According to Lambert (1973) and (Awoyemi, 1999 and 2001), a linear multi-step method of type (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) $\sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_{ij}$

One-step first derivative method

(i) Since the One-step first derivative method (10) 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 $\beta_{11} = \frac{1}{2}$

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

$= -1 + 1$
= 0

Also, the second condition is satisfied.

(iii) $\sum_{j=0}^{l} j\alpha_j = 0\alpha_0 + 1\alpha_1$ and

$$\sum_{j=0}^{l} \beta_{ij} = \beta_{10} + \beta_{11}$$

= 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.

One–step second derivative method

(i) The one – step second derivative method (14) 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 $\beta_{21} = -\frac{1}{2}$

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

Also the second condition is satisfied;

(iii) $\sum_{j=0}^{l} j\alpha_j = 0\alpha_0 + 1\alpha_1$ and

$$\sum_{j=0}^{l} \beta_{ij} = \beta_{10} + \beta_{11} + \beta_{20} + \beta_{21}$$

= 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.

Two–step first derivative method

(i) The Two – step second derivative method (19) 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.

Two – step second derivative method

(i) The two-step second derivative method (22) is of order 7, then the first condition is satisfied.

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

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

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

$$\sum_{j=0}^{2} \alpha_j = \alpha_0 + \alpha_1 + \alpha_2 = 1 - 2 + 1 = 0$$

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.

Zero – stability

According to Auzinger et al. (1992), Bakaev and Osterman (2002), Babatola and Ademiluyi (2007), a linear multistep method of the form:

$$y_{n+k} = \alpha_o y_n + h\left(\beta_1 y'_{n+k} + \beta_0 y'_n\right)$$

with first characteristic polynomial;

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

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

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:

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

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

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

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

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:

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

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

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

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

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.

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:

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

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

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

Solving gives $r = 0$ or $r = 1$(twice)
Since the roots are within a unit circle, the method is zero-stable.

Convergence

According to Palencia (1994) Auzinger et al. (1996) 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.

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. (Palencia,1993).To ascertain the region of A – stability of the methods, boundary locus method and Dalhquist Stability model test equation ($y' = \lambda y$) are adopted.

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:

$$|u(z)| < 1$$

that is., $\left|\frac{1 + z/2}{1 - z/2}\right| < 1$

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

Simplifying, we have sets A and B with;

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

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 1. Hence, the method is A – stable.

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 2.

Hence the method is A – stable.

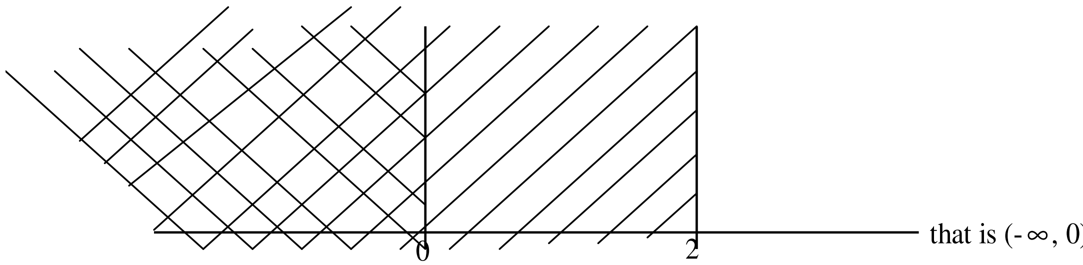

Figure 1. Region of absolute stability of one-step first derivative method.

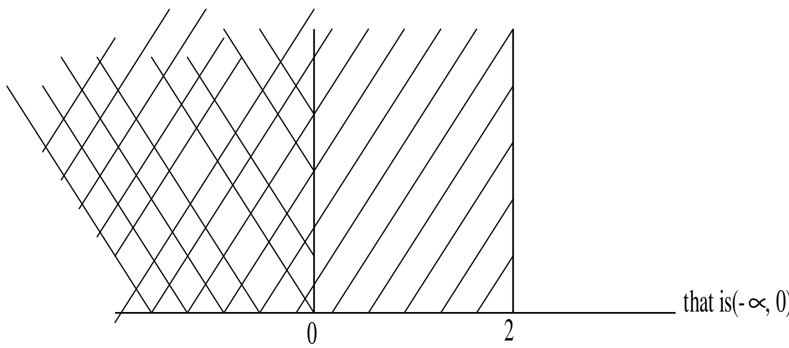

Figure 2. Region of absolute stability of one-step second derivative method.

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

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

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

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

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.

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:

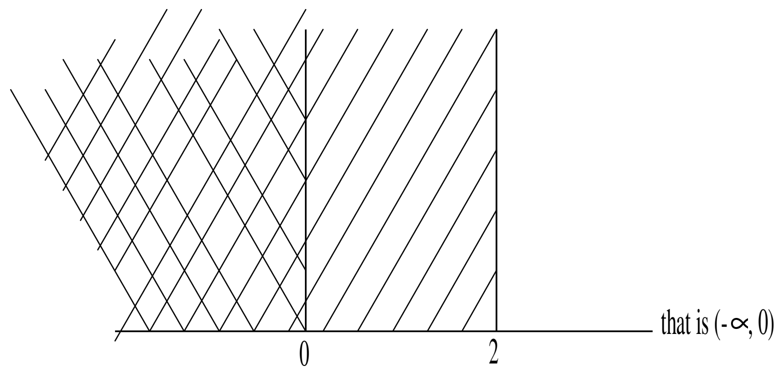

Figure 3. Region of absolute stability of two-step second derivative method. Hence the method is A – stable.

Table 1. Results obtained for problem 1 in respect of methods 1 to 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

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

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

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

Rationalizing, simplifying and considering only the real part of:

$$h(\theta)=x(\theta)+iy(\theta),\quad 0^0\le\theta\le180^0$$

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

the region of A – stability is shown by the doubly shaded portion of the region in Figure 3.

Test problems

To test the suitability and performance of the schemes, the formulae are translated into computer algorithms using FORTRAN programming language. These FORTRAN programmes are used to solve some sample first order initial value problems of (non-stiff and stiff) ODEs. The results are presented in Tables 1 to 4 and Figures 4 to 6. The main aim is to determine the accuracy of the methods as the order of the derivative and step number were increasing.

Problem 1

A non – stiff I. V. P.

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

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

Table 2. Results obtained for problem 2 in respect of methods 1 to 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 3. Results obtained for problem 3 in respect of methods 1 to 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	3.059023205D-08	3.059611237D-08	3.059062114D-08	3.059062066D-08	3.059023211D-08
0.2	6.118046410D-08	6.119936216D-08	6.118050163D-08	6.118050073D-08	6.118046493D-08
0.3	9.177069615D-08	9.179463292D-08	9.177096391D-08	9.177096122D-08	9.177069662D-08
0.4	1.223609282D-07	1.227323625D-07	1.223613532D-07	1.223613211D-07	1.223609312D-07
0.5	1.529511603D-07	1.534632604D-07	1.529520391D-07	1.529520113D-07	1.529511682D-07
0.6	1.835413923D-07	1.838360172D-07	1.835463520D-07	1.835463208D-07	1.835413984D-07
0.7	2.141316244D-07	2.148069141D-07	2.141324635D-07	2.141324341D-07	2.141316327D-07
0.8	2.447218564D-07	2.449721306D-07	2.447301651D-07	2.447301372D-07	2.447218587D-07
0.9	2.753129885D-07	2.758314022D-07	2.753243114D-07	2.753243049D-07	2.753129916D-07
1.0	3.059023205D-07	3.064125662D-07	3.059042916D-07	3.059042563D-07	3.059023246D-07

Table 4. Results obtained for problem 4 in respect of methods 1 to 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

Problem 2

A stiff I. V. P.

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

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

Problem 3

A stiff I. V. P.

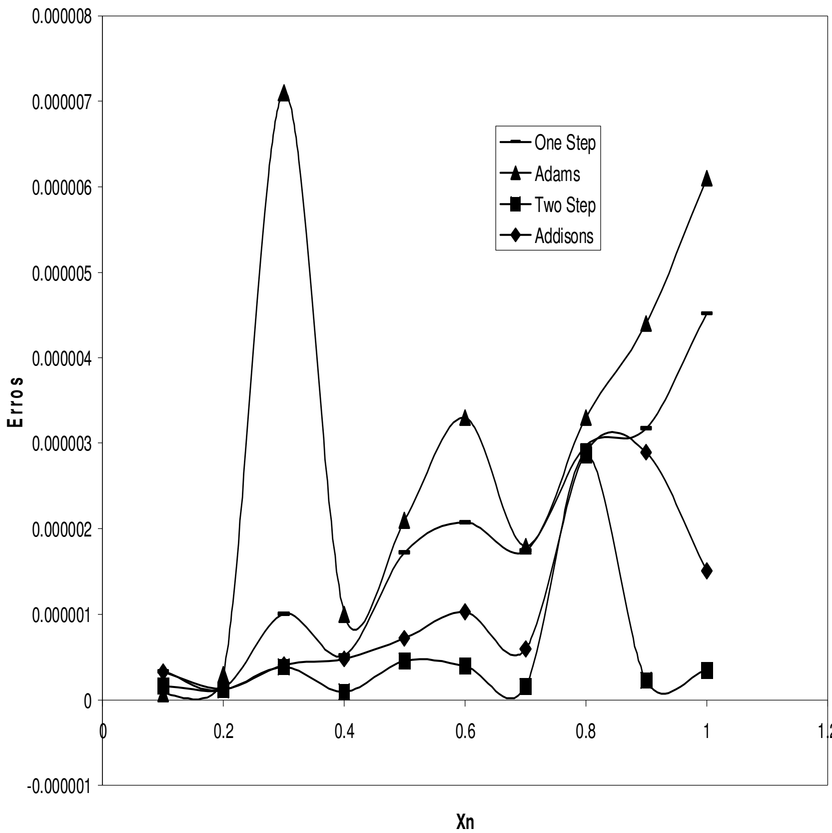

Figure 4. Errors of second derivative methods and some existing l mm with respect to problem one.

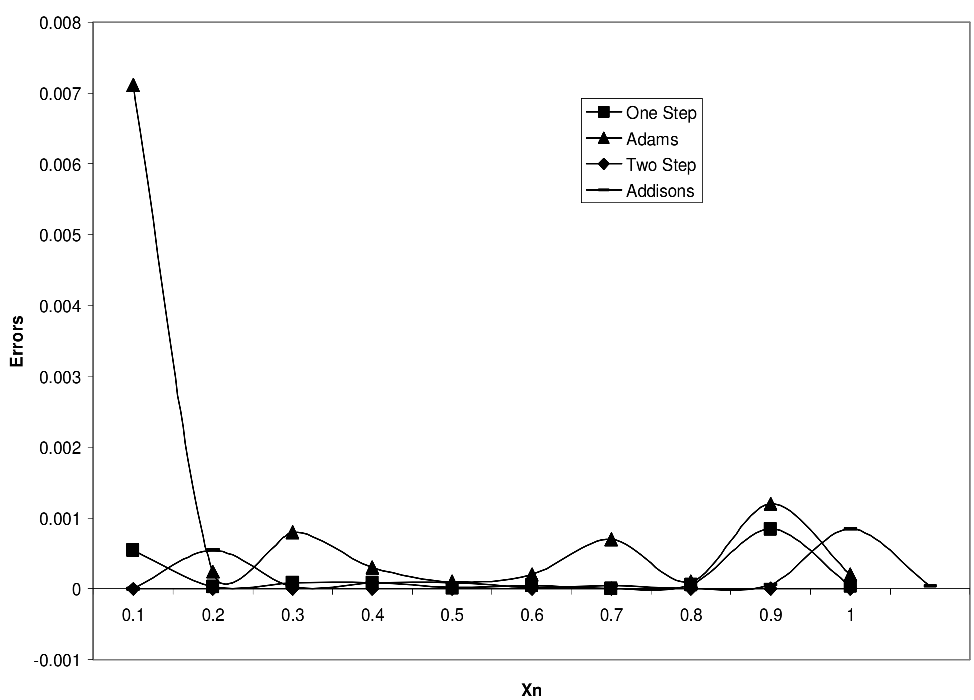

Figure 5. Errors of second derivative methods and some existing l mm with respect to problem two.

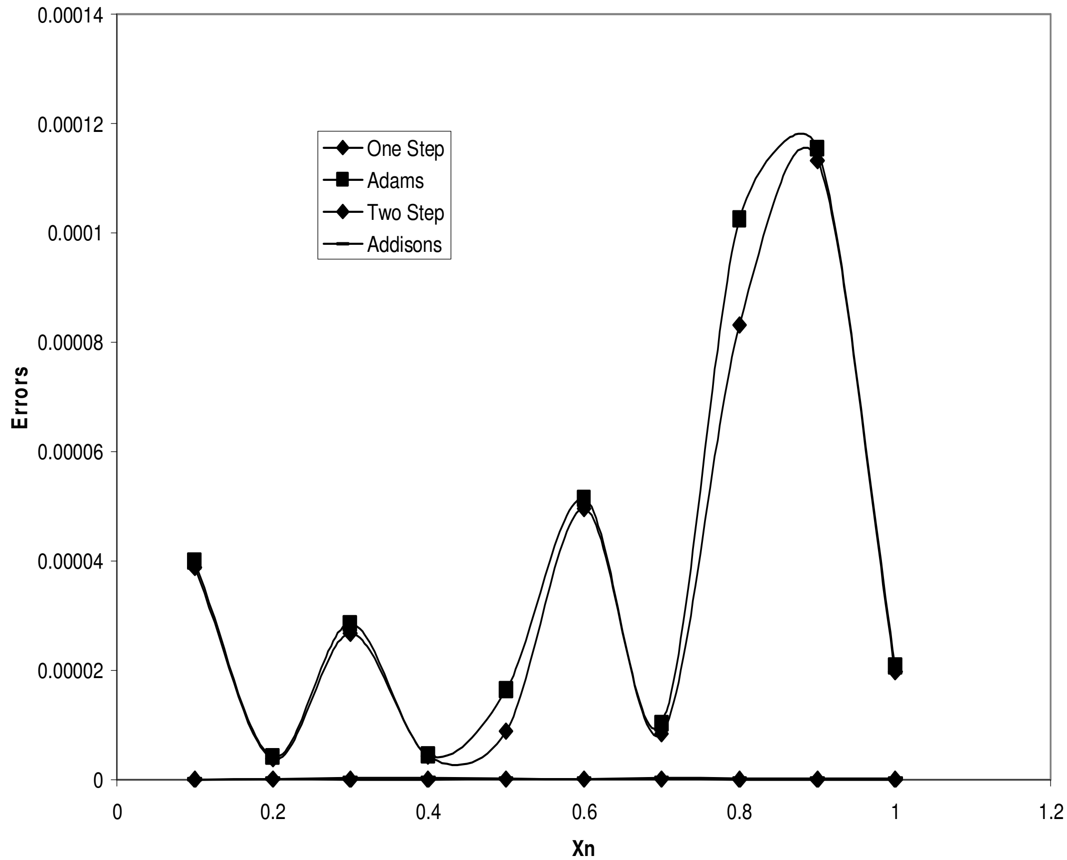

Figure 6. Errors of second derivative methods and some existing l mm with respect to problem three.

$$y' = -15y(x), \quad y(0) = 1 \text{ with } h = 0.1$$

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

Problem 4

A non-Linear I.V.P. (Bernoulli differential equation)

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

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

Conclusion

In this study, a class of implicit multi-derivative linear multi-step methods has 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 and that second derivative methods gave better accuracy than first derivative methods.

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