

AN OPTIMAL 6-STEP IMPLICIT LINEAR MULTISTEP METHOD FOR INITIAL VALUE PROBLEMS

*NDANUSA, A., & ADEBOYE, K. R.

Department of Mathematics, Federal University of Technology, Minna, Nigeria

*E-mail: as.ndanusa@futminna.edu.ng, profadeboye@gmail.com

Abstract

In this paper, we employ Taylor series expansion to develop a 6-step implicit linear multistep method of optimal order, for solving initial value problems. By assigning a suitable value to the free parameters involved, we develop a numerical scheme. Of course, many numerical schemes for solving differential equations abound. However, for a scheme to be of any practical value, a necessary condition for its acceptability is its convergence. Our scheme has thus satisfied the necessary and sufficient conditions for convergence; hence, its acceptability. More so, we apply the scheme to solve some practical problems involving differential equations. A comparison of results obtained with exact solutions will further establish the efficiency of this method.

Keywords: Initial Value Problem(IVP), Optimal, Implicit, Linear Multistep Method (LMM), Zero-Stability, Consistency, K-Step, Order

Introduction

The Cauchy's problem for the differential equation of the n th order

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

consists in finding the function $y = y(x)$ satisfying this equation and the initial conditions

$$y(x_0) = y_0, \quad y'(x_0) = y_0', \dots, y^{(n-1)}(x_0) = y_0^{(n-1)}, \quad (2)$$

where $x_0, y_0, y_0', \dots, y_0^{(n-1)}$ are the given numbers.

Cauchy's problem for a system of differential equations

$$\left. \begin{aligned} \frac{dy_1}{dx} &= f_1(x, y_1, y_2, \dots, y_n), \\ \frac{dy_2}{dx} &= f_2(x, y_1, y_2, \dots, y_n), \\ &\dots\dots\dots \\ \frac{dy_n}{dx} &= f_n(x, y_1, y_2, \dots, y_n), \end{aligned} \right\} \quad (3)$$

consists in finding the functions y_1, y_2, \dots, y_n satisfying this system and the initial conditions

$$y_1(x_0) = y_{10}, y_2(x_0) = y_{20}, \dots, y_n(x_0) = y_{n0} \quad (4)$$

A system containing higher-order derivatives and solved with respect to senior derivatives of the required functions by introducing new unknown functions can be reduced to the form (3). In particular, the differential equation of the n th order

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

is reduced to the form (3) with the aid of the substitution

$$y_1 = y', y_2 = y'', \dots, y_{n-1} = y^{(n-1)},$$

which gives the following system:

$$\begin{aligned} \frac{dy}{dx} &= y_1, \\ \frac{dy_1}{dx} &= y_2, \\ &\dots \end{aligned}$$

$$\begin{aligned}\frac{dy_{n-1}}{dx} &= y_{n-1}, \\ \frac{dy_n}{dx} &= f(x, y_1, y_2, \dots, y_{n-1}).\end{aligned}$$

If the general solution of equation (1) or system (3) is successfully found, then Cauchy's problem is reduced to finding the values of arbitrary constants. But it is rather difficult to find the exact solution of Cauchy's problem and it is successfully found only in rare cases; more often we have to solve Cauchy's problem using approximate methods by the application of numerical methods (Kopchenova and Maron, 1981).

Several studies on numerical methods for solving differential equations have been carried out including Ndanusa (2004), that derived a linear multistep method of order eight for solving IVPs. One outstanding feature of this method is that it has a considerable number of free parameters, the judicious use of which can produce schemes that have less function evaluations than usual at each step of the computation. Some later developments in this field include the works of Evans and Tremaine (1999), Galeone and Gerrappa (2006), Gerrappa (2009), Vlachos *et al.* (2009), Vigo-Aguiar and Simos (2001), Afolyan *et al.* (2012), Panopoulos *et al.* (2013) and Albi *et al.* (2020).

Materials and Methods

Derivation of Scheme: We consider the IVP (1) and initial conditions (2). Let y_n be an approximation to the theoretical solution at x_n , that is, to $y(x_n)$, and let $f_n = f(x_n, y_n)$. Then, we say a linear multistep method (Imm) of step number k , or a linear k -step method is a computational method for determining, the sequence $\{y_n\}$ that takes the form of a linear relationship between y_{n+j} and f_{n+j} , $j = 0, 1, \dots, k$. Thus the general Imm may be written.

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \sum_{j=0}^k \beta_j f_{n+j} \quad (5)$$

Where α_j and β_j are constants; we assume $\alpha_k = 1$ and that not both α_0 and β_0 are zero. We say that the method is explicit if $\beta_k = 0$, and implicit if $\beta_k \neq 0$ (Lambert, 1973).

We employ the method of Taylor expansions as outlined by Lambert (1973) to derive our 6-step method of order 8 thus.

Let ℓ be the linear difference operator defined by

$$\ell[y(t); h] = \sum_{j=0}^k [\alpha_j y(t+jh) - h\beta_j y'(t+jh)] \quad (6)$$

where $y(t)$ is an arbitrary function, continuously differentiable on $[a, b]$. if we expand $y(t+jh)$ and its derivative $y'(t+jh)$ as Taylor series about t , and collecting like terms we have

$$\ell[y(t); h] = c_0 y(t) + c_1 h y'(t) + c_2 h^2 y''(t) + \dots + c_q h^q y^{(q)}(t) + \dots \quad (7)$$

where c_q are constants.

Suppose we choose to expand $y(t+jh)$ and $y'(t+jh)$ about $t+rh$, where r need not necessarily be an integer. We obtain

$$\ell[y(t); h] = D_0 y(t+rh) + D_1 h y'(t+rh) + \dots + D_q h^q y^{(q)}(t+rh) \quad (8)$$

If we employ the Taylor expansions

$$y^{(q)}(t + rh) = y^{(q)}(t) + rhy^{(q+1)}(t) + \dots + \frac{r^s h^s}{s!} y^{(q+s)}(t) + \dots$$

$$q = 0, 1, 2, \dots$$

where $y^{(0)}(t) = y(t)$; and substitute in (8), we obtain on equating term by term with (7)

$$\left. \begin{aligned} c_0 &= D_0 \\ c_1 &= D_1 + rD_0 \\ c_2 &= D_2 + rD_1 + \frac{r^2}{2!} D_0 \\ &\vdots \\ c_p &= D_p + rD_{p-1} + \dots + \frac{r^p}{p!} D_0 \\ c_{p+1} &= D_{p+1} + rD_p + \dots + \frac{r^{p+1}}{(p+1)!} D_0 \end{aligned} \right\} \quad (9)$$

It follows that $c_0 = c_1 = \dots c_p = 0$ iff $D_0 = D_1 = \dots D_p = 0$

The formulae for the constants D_q expressed in terms of α_j, β_j are

$$\left. \begin{aligned} D_0 &= \alpha_0 + \alpha_1 + \alpha_2 + \dots + \alpha_k \\ D_1 &= -r\alpha_0 + (1-r)\alpha_1 + (2-r)\alpha_2 + \dots + (k-r)\alpha_k \\ &\quad -(\beta_0 + \beta_1 + \beta_2 + \dots + \beta_k) \\ &\vdots \\ D_q &= \frac{1}{q!} [(-r)^q \alpha_0 + (1-r)^q \alpha_1 + (2-r)^q \alpha_2 + \dots + (k-r)^q \alpha_k] \\ &\quad - \frac{1}{(q-1)!} [(-r)^{q-1} \beta_0 + (1-r)^{q-1} \beta_1 + \dots + (k-r)^{q-1} \beta_k], \\ &\quad q = 2, 3, \dots \end{aligned} \right\} \quad (10)$$

Consistency demands that,

$$\rho(1) = 0 \quad \text{and} \quad \rho'(1) = \sigma(1) \quad (11)$$

where,

$$\rho(\xi) = \sum_{j=0}^k \alpha_j \xi^j \quad (12)$$

and

$$\sigma(\xi) = \sum_{j=0}^k \beta_j \xi^j \quad (13)$$

are called the first and second characteristic polynomials of (5) respectively.

The Imm (5) is said to be zero-stable if no root of (12) has modulus greater than one, and if every root with modulus one is simple.

Our goal is to derive a 6-step method of optimal order (i.e. order 8). It implies all the roots of the first characteristic polynomial must lie on the unit circle. We know that $\rho(\xi)$ is a

polynomial of degree 6. Hence, by consistency, it has one real root at +1 and another real root at -1. The four remaining roots must be complex.

Hence we have

$$\xi_1 = +1, \xi_2 = -1, \xi_3 = e^{i\theta_1}, \xi_4 = e^{-i\theta_1}, \xi_5 = e^{i\theta_2}, \xi_6 = e^{-i\theta_2}$$

Hence

$$\left. \begin{aligned} \alpha_6 &= +1, & \alpha_5 &= -2(a+b), & \alpha_4 &= (4ab+1), & \alpha_3 &= 0, \\ \alpha_2 &= -(4ab+1), & \alpha_1 &= 2(a+b), & \alpha_0 &= -1 \end{aligned} \right\} \quad (14)$$

We now state the order requirement in terms of the coefficients D_q .

$$D_0 = \alpha_0 + \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 + \alpha_5 + \alpha_6$$

$$D_1 = -r\alpha_0 + (1-r)\alpha_1 + (2-r)\alpha_2 + (3-r)\alpha_3 + (4-r)\alpha_4 + (5-r)\alpha_5 + (6-r)\alpha_6$$

$$-(\beta_0 + \beta_1 + \beta_2 + \beta_3 + \beta_4 + \beta_5 + \beta_6)$$

...

...

...

$$D_8 = \frac{1}{8!} [(-r)^8\alpha_0 + (1-r)^8\alpha_1 + (2-r)^8\alpha_2 + (3-r)^8\alpha_3 + (4-r)^8\alpha_4 + (5-r)^8\alpha_5 + (6-r)^8\alpha_6]$$

$$-\frac{1}{7!} [(-r)^7\beta_0 + (1-r)^7\beta_1 + (2-r)^7\beta_2 + (3-r)^7\beta_3 + (4-r)^7\beta_4 + (5-r)^7\beta_5 + (6-r)^7\beta_6]$$

$$D_9 = \frac{1}{9!} [(-r)^9\alpha_0 + (1-r)^9\alpha_1 + (2-r)^9\alpha_2 + (3-r)^9\alpha_3 + (4-r)^9\alpha_4 + (5-r)^9\alpha_5 + (6-r)^9\alpha_6]$$

$$-\frac{1}{8!} [(-r)^8\beta_0 + (1-r)^8\beta_1 + (2-r)^8\beta_2 + (3-r)^8\beta_3 + (4-r)^8\beta_4 + (5-r)^8\beta_5 + (6-r)^8\beta_6]$$

Setting $r = 3$ and $D_q = 0$, $q = 2, 3, 4, 5, 6, 7, 8$ we have,

$$D_2 = \frac{1}{2!} [3^2\alpha_0 + 2^2\alpha_1 + \alpha_2 + \alpha_4 + 2^2\alpha_5 + 3^2\alpha_6] - [-3\beta_0 - 2\beta_1 - \beta_2 + \beta_4 + 2\beta_5 + 3\beta_6] = 0$$

$$D_3 = \frac{1}{3!} [-3^3\alpha_0 - 2^3\alpha_1 - \alpha_2 + \alpha_4 + 2^3\alpha_5 + 3^3\alpha_6] - \frac{1}{2!} [3^2\beta_0 + 2^2\beta_1 + \beta_2 + \beta_4 + 2^2\beta_5 + 3^2\beta_6] = 0$$

$$D_4 = \frac{1}{4!} [3^4\alpha_0 + 2^4\alpha_1 + \alpha_2 + 2^4\alpha_5 + 3^4\alpha_6] - \frac{1}{3!} [3^3\beta_0 + 2^3\beta_1 - \beta_2 + \beta_4 + 2^3\beta_5 + 3^3\beta_6] = 0$$

$$D_5 = \frac{1}{5!} [-3^5\alpha_0 - 2^5\alpha_1 - \alpha_2 + \alpha_4 + 2^5\alpha_5 + 3^5\alpha_6] - \frac{1}{4!} [3^4\beta_0 + 2^4\beta_1 + \beta_2 + \beta_4 + 2^4\beta_5 + 3^4\beta_6] = 0$$

$$D_6 = \frac{1}{6!} [3^6\alpha_0 + 2^6\alpha_1 + \alpha_2 + \alpha_4 + 2^6\alpha_5 + 3^6\alpha_6] - \frac{1}{5!} [-3^5\beta_0 - 2^5\beta_1 - \beta_2 + \beta_4 + 2^5\beta_5 + 3^5\beta_6] = 0$$

$$D_7 = \frac{1}{7!} [-3^7\alpha_0 - 2^7\alpha_1 - \alpha_2 + \alpha_4 + 2^7\alpha_5 + 3^7\alpha_6] - \frac{1}{6!} [3^6\beta_0 + 2^6\beta_1 + \beta_2 + \beta_4 + 2^6\beta_5 + 3^6\beta_6] = 0$$

$$D_8 = \frac{1}{8!} [3^8\alpha_0 + 2^8\alpha_1 + \alpha_2 + \alpha_4 + 2^8\alpha_5 + 3^8\alpha_6] - \frac{1}{7!} [-3^7\beta_0 - 2^7\beta_1 - \beta_2 + \beta_4 + 2^7\beta_5 + 3^7\beta_6] = 0$$

However, on inserting the values we have obtained for the α_j into these equations we have

$$\left. \begin{aligned}
-3\beta_0 - 2\beta_1 - \beta_2 + \beta_4 + 2\beta_5 + 3\beta_6 &= 0 \\
3^2\beta_0 + 2^2\beta_1 + \beta_2 + \beta_4 + 2^2\beta_5 + 3^2\beta_6 &= \frac{2}{3}[28 + 4ab - 16(a + b)] \\
-3^3\beta_0 + 2^3\beta_1 - \beta_2 + \beta_4 + 2^3\beta_5 + 3^3\beta_6 &= 0 \\
3^4\beta_0 + 2^4\beta_1 + \beta_2 + \beta_4 + 2^4\beta_5 + 3^4\beta_6 &= \frac{2}{5}[244 + 4ab - 64(a + b)] \\
-3^5\beta_0 - 2^5\beta_1 - \beta_2 + \beta_4 + 2^5\beta_5 + 3^5\beta_6 &= 0 \\
3^6\beta_0 + 2^6\beta_1 + \beta_2 + \beta_4 + 2^6\beta_5 + 3^6\beta_6 &= \frac{2}{7}[2188 + 4ab - 256(a + b)] \\
-3^7\beta_0 - 2^7\beta_1 - \beta_2 + \beta_4 + 2^7\beta_5 + 3^7\beta_6 &= 0
\end{aligned} \right\} \quad (15)$$

We can satisfy the first, third, fifth and seventh of these equations if we choose

$$\beta_2 = \beta_4, \beta_1 = \beta_5, \beta_0 = \beta_6$$

The remaining three equations give

$$3^2\beta_0 + 2^2\beta_1 + \beta_2 = \frac{1}{3}[28 + 4ab - 16(a + b)] \quad (16)$$

$$3^4\beta_0 + 2^4\beta_1 + \beta_2 = \frac{1}{5}[244 + 4ab - 64(a + b)] \quad (17)$$

$$3^6\beta_0 + 2^6\beta_1 + \beta_2 = \frac{1}{7}[2188 + 4ab - 256(a + b)] \quad (18)$$

Solving the above set of equations give

$$\left. \begin{aligned}
\beta_0 &= \frac{1}{945}[278 + 5ab + 16(a + b)] = \beta_6 \\
\beta_1 &= \frac{1}{105}[160 - 8ab - 76(a + b)] = \beta_5 \\
\beta_2 &= \frac{1}{105}[62 + 167ab - 272(a + b)] = \beta_4
\end{aligned} \right\} \quad (19)$$

Finally, solving $D_1 = 0$ gives

$$\beta_3 = \frac{1}{945}(3008 + 5688ab - 1328(a + b)) \quad (20)$$

We solve for the error constant, D_9

$$\begin{aligned}
D_9 &= \frac{1}{9!}[-3^9\alpha_0 - 2^9\alpha_1 - \alpha_2 + \alpha_4 + 2^9\alpha_5 + 3^9\alpha_6] - \frac{1}{8!}[3^8\beta_0 + 2^8\beta_1 + \beta_2 + \beta_4 + 2^8\beta_5 + 3^8\beta_6] \\
D_9 &= -\frac{1}{907200}[6016 + 736ab - 8576(a + b)] \quad (21)
\end{aligned}$$

Since $a = \cos \theta_1, b = \cos \theta_2, 0 < \theta_1 < \pi, 0 < \theta_2 < \pi$, a and b are restricted to the range $-1 < a < 1$ and $-1 < b < 1$.

Our choice of values for a and b is guided by the fact that we like to minimize the error constant as well as the need to develop a method that makes computation easier by reducing the number of operations involved. We assign the following values to the free variables a and b .

$$a = 1/2, b = -1/2$$

This causes four coefficients $\alpha_1, \alpha_2, \alpha_4$ and α_5 , to vanish. Thus we have the following values for the coefficients α_i, β_i .

$$\alpha_6 = +1, \alpha_5 = 0, \alpha_4 = 0, \alpha_3 = 0, \alpha_2 = 0, \alpha_1 = 0, \alpha_0 = -1$$

$$\beta_0 = \frac{41}{140} = \beta_6, \beta_1 = \frac{162}{105} = \beta_5, \beta_2 = \frac{27}{140} = \beta_4, \beta_3 = \frac{68}{35}$$

The error constant is obtained from equation (21) as: -0.006428571429.

Thus, our scheme is as follows:

$$y_{n+6} - y_n = h \left[\frac{41}{140} f_{n+6} + \frac{162}{105} f_{n+5} + \frac{27}{140} f_{n+4} + \frac{68}{35} f_{n+3} + \frac{27}{140} f_{n+2} + \frac{162}{105} f_{n+1} + \frac{41}{140} f_n \right] \quad (22)$$

Convergence Analysis

For the scheme (22) to be convergent, we establish the following:

$$\begin{aligned} \rho(\xi) &= \sum_{j=0}^6 \alpha_j \xi^j = \xi^6 - 1 \\ \rho(1) &= 1 - 1 = 0 \\ \rho'(\xi) &= 6\xi^5 \\ \rho'(1) &= 6(1) = 6 \\ \sigma(\xi) &= \sum_{j=0}^6 \beta_j \xi^j = \frac{41}{140} \xi^6 + \frac{162}{105} \xi^5 + \frac{27}{140} \xi^4 + \frac{68}{35} \xi^3 + \frac{27}{140} \xi^2 + \frac{162}{105} \xi + \frac{41}{140} \\ \sigma(1) &= \frac{41}{140} + \frac{162}{105} + \frac{27}{140} + \frac{68}{35} + \frac{27}{140} + \frac{162}{105} + \frac{41}{140} = 6 \end{aligned}$$

Hence the scheme is consistent.

Next, we find the roots of $\rho(\xi)$:

$$\rho(\xi) = \xi^6 - 1 = 0$$

And we have the following as its roots:

$$\begin{aligned} \xi_1 &= +1; \xi_2 = -1; \xi_3 = \frac{1 + \sqrt{3}}{2} i \\ \xi_4 &= \frac{1 - \sqrt{3}}{2} i; \xi_5 = \frac{-1 + \sqrt{3}}{2} i; \xi_6 = \frac{-1 - \sqrt{3}}{2} i \end{aligned}$$

It is obvious that $|\xi_i| \leq 1$, $i = 1, 2, 3, 4, 5, 6$.

Thus $\zeta_i, i = 1, 2, \dots, 6$ satisfy the zero stability condition. Hence, we conclude the scheme is convergent.

Results and Discussion

Tables 1 and 2 show the results obtained when the scheme is applied to solve some differential equation problems. The results of such computations is compared with the exact solutions as well.

Table 1: *PROBLEM: $F = (1 + Y)/(2 + X); Y(0) = 1; h = 0.1$*
EXACTSOLUTION: $Y(X) = 2 + X - 1$

x	EXACT	$y(x)$	ERROR
0.0	1.0000000000	1.0000000000	0.0000000000E+00
0.1	1.1000000000	1.1000000000	0.0000000000E+00
0.2	1.2000000000	1.2000000000	0.0000000000E+00
0.3	1.3000000000	1.3000000000	0.0000000000E+00
0.4	1.4000000000	1.4000000000	0.0000000000E+00
0.5	1.5000000000	1.5000000000	0.0000000000E+00
0.6	1.6000000000	1.6000000000	0.0000000000E+00
0.7	1.7000000000	1.7000000000	0.0000000000E+00
0.8	1.8000000000	1.8000000000	0.0000000000E+00
0.9	1.9000000000	1.9000000000	0.0000000000E+00
1.0	2.0000000000	2.0000000000	0.0000000000E+00

TABLE 2: *PROBLEM: $F = X^5 + 2X^4 + 3X^3; Y(0) = 1; h = 0.1$*
EXACTSOLUTION: $Y(X) = (X^6/6) + (2X^5/5) + (3X^4/4) + 1$

x	EXACT	$y(x)$	ERROR
0.0	1.0000000000	1.0000000000	0.0000000000E+00
0.1	1.0000791667	1.0000793542	1.8749999997E-07
0.2	1.0013386667	1.0013390833	4.1666666672E-07
0.3	1.0071685000	1.0071691875	6.8750000004E-07
0.4	1.0239786667	1.0239796667	9.9999999992E-07
0.5	1.0619791667	1.0619805208	1.3541666666E-06
0.6	1.1360800000	1.1360800000	0.0000000000E+00
0.7	1.2669111667	1.2669111667	0.0000000000E+00
0.8	1.4819626667	1.4819626667	0.0000000000E+00
0.9	1.8168445000	1.8168445000	0.0000000000E+00
1.0	2.3166666667	2.3166666667	0.0000000000E+00

As expected, the scheme exhibits high accuracy in Table 1. This is due to the fact that the solution of the differential equation is a polynomial of degree one. This trend is also visible in Table 2. This is according to expectation as well; since the solution of the differential equation is a polynomial of degree six and the scheme is a 6-step method of order 8.

Conclusion

The results of convergence analysis established, theoretically, that the scheme is convergent. More so, the results of practical application of the scheme to sample problems as exhibited in Tables 1 and 2 goes further to validate the convergence analysis. Therefore, it is sufficient to conclude that our 6-step implicit linear multistep method of order 8 is accurate, effective, efficient, and acceptable as a numerical method for solving initial value problems.

References

- Afolyan, I., Anastassi, Z. A., & Simos, T. E. (2012). A new family of symmetric linear four-step methods for the efficient integration of the Schrödinger equation and related oscillatory problems. *Applied Mathematics and Computation*. 218(9), 5370- 5382.

- Albi, G., Dimarco, G., & Pareschi, L. (2020). Implicit-explicit multistep methods for hyperbolic systems with multiscale relaxation. *SIAM Journal on Scientific Computing*. 42(4): A2402–A2435.
- Evans, N. W., & Tremaine, S. (1999). Linear multistep methods for integrating reversible differential equations. *The Astronomical Journal*, 118(4), 1888-1899
- Gerrappa, R. (2009). On some explicit Adams multistep methods for fractional differential equations. *Journal of Computational and Applied Mathematics*. 229(2), 392-399.
- Galeone, L., & Gerrappa, R. (2006). On multistep methods for differential equations of fractional order. *Mediterranean Journal of Mathematics*, 3(3-4), 565-580.
- Kopchenova, N. V., & Maron, I. A. (1981). *Computational mathematics*. Moscow: MIR Publishers. Pp. 198-199.
- Lambert, J. D. (1973). *Computational methods in ordinary differential equations*. NY: John Wiley. Pp. 12, 23-24.
- Ndanusa, A. (2004). Derivation and application of a linear multistep numerical Scheme. *Leonardo Journal of Sciences*, 10, 9-16.
- Panopoulos, G. A., Anastassi, Z. A., & Simos, T. E. (2013). A new eight-step symmetric embedded predictor-corrector method (EPCM) for orbital problems and related IVPs with oscillatory solutions. *The Astronomical Journal*, 145(3), 1-9.
- Vigo-Aguiar, J., & Simos, T. E. (2001). An exponentially fitted and trigonometrically fitted method for the numerical solution of orbital problems. *The Astronomical Journal*, 122(3), 1656-1660.
- Vlachos, D. S., Anastassi, Z. A., & Simos, T. E. (2009). A new family of multistep methods with improved phase-lag characteristics for the integration of orbital problems. *The Astronomical Journal*, 138(1), 86-94.