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Variable Step-size Implementation of Hybrid Linear Multistep Methods

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Abstract

This paper describes the construction of third derivative hybrid linear multistep method (TDHLMM) which is A-stable for step number $k=1$ ***and*** $A(\alpha)$ ***-stable for*** $k=2(1)6$. ***Numerical results are given to show the accuracy and efficiency of the new scheme..***

Keywords: Hybrid method, Backward Differentiation Formulas, Collocation, Interpolation, Second Order, Multiple Finite Difference.

1.0 Introduction

This paper introduces a class of third derivative hybrid LMM for the numerical solution of stiff (IVPs) in ordinary differential equations (ODEs)

$$y' = f(x,y), \;\; y(x_0)=y_0, \quad a \le x \le b. \tag{1}$$

Third derivative multistep methods (TDMM) were first proposed by Ezzeddine and Hojjati [1] but not in hybrid mode. The TDMM was observed to be $A(\alpha)$-stable for $k \le 5$ and unstable when $k \ge 6$. Recently, Okuonghae and Ikhile [2] introduced third derivative hybrid LMM

$$\begin{cases} y(x_n+vh) = \sum_{j=0}^{k} \alpha_j(v) y_{n+j} + h\eta_k(v) f_{n+k} + h^2 \delta_k(v) f'_{n+k} \\ y(x_n+th) = y_{n+k-1} + h\sum_{j=0}^{k} \beta_j(t,v) f_{n+j} + h\varphi_v(t,v) f_{n+v} + h^2 \eta_k(t,v) f'_{n+k} + h^3 l_k(t,v) f''_{n+k} \end{cases} \tag{2}$$

for stiff IVPs. Investigation shows that the methods (2) are*A*-stable for step number $k \le 4$ and $A(\alpha)$-stable for step number $k = 5(1)13$. The new hybrid linear multistep method (hereafter referred to as TDHLMM) for the numerical solution of (1) is

$$\begin{cases} y_{n+v} = \sum_{j=0}^{k} \alpha_j(v) y_{n+j} + h\beta_k(v) f_{n+k} & (3a) \\ y(x_n+th) = y_{n+k-1} + h\sum_{j=0}^{k} \beta_j(t,v) f_{n+j} + h^2 \varphi_v(t,v) f'_{n+v} + h^3 \gamma_v(t,v) f''_{n+v} & (3b) \end{cases}$$

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The continuous coefficients $\alpha_k(t)$, $\alpha_{k-1}(t)$ and $\alpha_v(v)$ are assumed to be one. Historically, hybrid LMM was first proposed independently by the authors in [3], [4] and [5] respectively.These hybrid LMM introduced an additional term to LMM. This term is a derivative at an off-step point, in the manner of RungeKutta methods. By doing this, Dahlquist's order barrier [9] for LMM can be broken. Examples of hybrid LMM are in [6, 7, 8, 9, 10, 11-17]. Practically, we compute the value of $f^{/}_{n+v}$ and $f^{//}_{n+v}$ in (3b) using the hybrid predictor, y_{n+v} in (3a) at point x_{n+v}. This paper is organized as follows: Section 2 is on the derivation of the third derivative hybrid LMM (TDHLMM). In section 3 we discuss the stability of the methods while in section 4 we give results arising from the numerical experiments.

2.0 The derivation of the methods

To derive the method in (3) we use the polynomial interpolant

$$\sum_{j=0}^{N} a_j x^j \qquad (4)$$

where $\{a_j\}_{j=0}^{N}$ are constant parameter to be determined. Here, $x = x_n + th$. Differentiating (4) with respect to *x* gives

$$y'(x) = f(x,y) = \sum_{j=1}^{N} j a_j x^{j-1}, \quad y''(x) = f'(x,y) = \sum_{j=2}^{N} j(j-1) a_j x^{j-2}, \quad y'''(x) = f''(x,y) = \sum_{j=3}^{N} j(j-1)(j-2) a_j x^{j-3} \qquad (5)$$

Collocating (5) at $x = x_{n+j}$, $j = 0(1)N$ and interpolating (4) at $x = x_{n+k-1}$ result in system of linear equations

$$\begin{pmatrix} 1 & x_{n+k-1} & x^2_{n+k-1} & . & . & x^N_{n+k-1} \\ 0 & 1 & 2x_n & . & . & Nx_n^{N-1} \\ . & . & . & . & . & . \\ 0 & 1 & 2x_{n+k} & . & . & Nx^{N-1}_{n+k} \\ 0 & 0 & 2 & . & . & N(N-1)x^{N-2}_{n+v} \\ 0 & 0 & 0 & . & . & N(N-1)(N-2)x^{N-3}_{n+v} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ . \\ . \\ . \\ a_N \end{pmatrix} = \begin{pmatrix} y_{n+k-1} \\ f_n \\ .. \\ f_{n+k} \\ f'_{n+v} \\ f''_{n+v} \end{pmatrix}. \qquad (6)$$

Solving (6) for $\{a_j\}_{j=0}^{N}$ and substitute the resulting expression into (4) yields the continuous scheme for a specified step number *k* [11-17]. Fixing $t = k$ and $v = k - \frac{1}{2}$ into the resulting continuous scheme gives the discrete scheme. The discrete coefficients of the hybrid LMM in (3) are given in Table 1 for $k = 1, 2, ..., 6$.

Table1: Coefficients of TDHLMM, $t = k, v = k - \frac{1}{2}$

k	1	2	3	4	5	6
γ_v	$\frac{-1}{12}$	$\frac{-11}{100}$	$\frac{269}{4110}$	$\frac{-18070}{304311}$	$\frac{-159406}{2921079}$	$\frac{-3040908}{600396435}$
ϕ_v	0	$\frac{3}{25}$	$\frac{24}{137}$	$\frac{20892}{101437}$	$\frac{93920}{417297}$	$\frac{85650296}{360237861}$
β_0	$\frac{1}{2}$	$\frac{-1}{100}$	$\frac{9}{5480}$	$\frac{-11881}{24344880}$	$\frac{273611}{1402117920}$	$\frac{-376791403}{4034664043200}$
β_1	$\frac{1}{2}$	$\frac{16}{25}$	$\frac{-25}{1096}$	$\frac{65087}{12172440}$	$\frac{-967583}{467372640}$	$\frac{1545658423}{1512999016200}$
β_2	0	$\frac{37}{100}$	$\frac{3923}{5480}$	$\frac{-37599}{1014370}$	$\frac{2648371}{233686320}$	$\frac{-1457017753}{268977602880}$
β_3	0	0	$\frac{1673}{5480}$	$\frac{9324137}{12172440}$	$\frac{-5237041}{100151280}$	$\frac{996320959}{50433300540}$
β_4	0	0	0	$\frac{6480689}{24344880}$	$\frac{375279857}{467372640}$	$\frac{-165254447047}{2420798425920}$
β_5	0	0	0	0	$\frac{22422389}{93474528}$	$\frac{139892479087}{168111001800}$
β_6	0	0	0	0	0	$\frac{891073248707}{4034664043200}$

Table 2: Coefficients of the hybrid predictor in (3), $v = k - \frac{1}{2}$

k	1	2	3	4	5	6
β_k	$-\frac{1}{4}$	$-\frac{3}{16}$	$-\frac{5}{32}$	$-\frac{35}{256}$	$-\frac{63}{512}$	$-\frac{231}{2048}$
α_0	$\frac{1}{4}$	$-\frac{1}{32}$	$\frac{1}{96}$	$-\frac{5}{1024}$	$\frac{7}{2560}$	$-\frac{7}{4096}$
α_1	$\frac{3}{4}$	$\frac{3}{8}$	$-\frac{5}{64}$	$\frac{7}{192}$	$-\frac{45}{2048}$	$\frac{77}{5120}$
α_2	0	$\frac{21}{32}$	$\frac{15}{32}$	$-\frac{35}{256}$	$\frac{21}{256}$	$-\frac{495}{8192}$
α_3	0	0	$\frac{115}{192}$	$\frac{35}{64}$	$-\frac{105}{512}$	$\frac{77}{512}$
α_4	0	0	0	$\frac{1715}{3072}$	$\frac{315}{512}$	$-\frac{1155}{4096}$
α_5	0	0	0	0	$\frac{5397}{10240}$	$\frac{693}{1024}$
α_6	0	0	0	0	0	$\frac{20559}{40960}$

The error constants $C_{p+1,1}^{(k)}$, $C_{p+1,2}^{(k)}$, and the order $p = k+1,\ p = k+4$ arising from the hybrid LMM are given from the local truncation error operator

$$\ell_1[y(x);\ h] = y(x_n + vh) - \sum_{j=0}^{k} \alpha_j(v) y(x_n + jh) + h\beta_k(v) y'(x_n + kh)$$
$$= C_{p+1,1}^{(k)} h^{k+1} y^{k+1}(x_n) + 0\left(h^{k+2}\right),$$

$$\ell_2[y(x);\ h] = y(x_n + th) - y(x_n + (k-1)h) + h\sum_{j=0}^{k} \beta_j(t,v) y'(x_n + jh) + h^2\phi_v(t,v) y''(x_n + vh)$$
$$+ h^3\gamma_v(t,v) y'''(x_n + vh) = C_{p+1,2}^{(k)} h^{k+4} y^{k+4}(x_n) + 0\left(h^{k+5}\right).$$

3.0 Stability Analysis of the TDHLMM

Definition 1: [17]. A numerical integrator is said to be *A*-stable if its region of absolute stability *R* incorporates the entire left half $\not\subset$ of the complex plane $\not\subset$, i.e.,

$$R = \left\{ z \in \not\subset \middle| \operatorname{Re}(z) < 0 \right\}.$$

Definition 2: [18]. A numerical integration scheme is said to be $A(\alpha)-stable$ for some $\alpha \in [0, \pi/2]$ if the wedge $S_\alpha = \{z : |Arg(-z)| < \alpha,\ z \neq 0\}$ is contained in its region of absolute stability. The largest $\alpha_{\max}$ is called the angle of absolute stability or the argument of stability.

Applying the scheme (3) to the scalar test problem $y' = \lambda y$ yields

$$\pi(w,z) = w^k - w^{k-1} - z\sum_{j=0}^{k}\beta_j w^j - z^2\varphi_v\left(\sum_{j=0}^{k}\alpha_j w^j + z\beta_k w^k\right) - z^3\gamma_v\left(\sum_{j=0}^{k}\alpha_j w^j + z\beta_k w^k\right). \qquad (7)$$

We investigate the zero-stability of the methods and found that the roots of the first characteristics polynomial $\pi(w,0) = 0$ are less than one. The plot of the roots of the stability polynomial (7) shows that the method (3) is A-stable for $k = 1$ and $A(\alpha)$-stable for $k = 2(1)6$, see Fig. 1. Table 3a gives the stability properties of the TDHLMM while Table 3b depicts the stability properties of the TDMM discussed in [1].

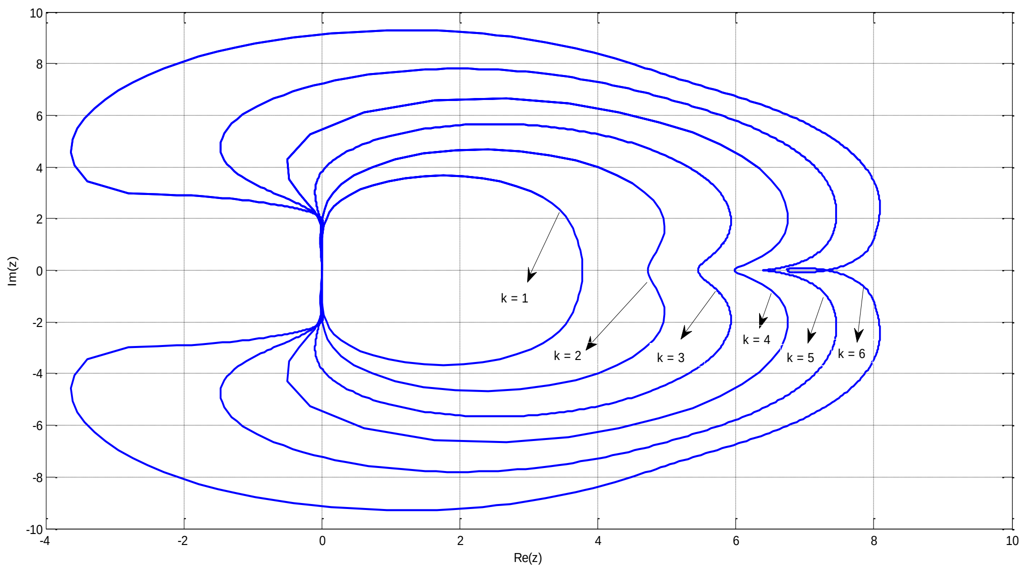

Fig. 1: The stability region of the TDHLMM.

Table 3a: Stability characteristics and error constants of the TDHLMM

K	1	2	3	4	5	6
P(3a)	2	3	4	5	6	7
P(3b)	4	5	6	7	8	9
Error Constant (3a)	$\frac{1}{48}$	$\frac{1}{128}$	$\frac{1}{256}$	$\frac{7}{3072}$	$\frac{3}{2048}$	$\frac{33}{32768}$
Error Constant (3b)	$\frac{-1}{480}$	$\frac{-9}{16000}$	$\frac{-11881}{55238400}$	$\frac{-27364}{272662650}$	$\frac{-376791403}{7066674318600}$	$\frac{-14437100734}{46479329776640}$
α	90^0	89.9^0	85^0	62^0	56^0	30^0

Table 3b: Stability characteristics and error constants of the TDMM [1]

k	1	2	3	4	5
P[1]	4	5	6	7	8
Error Constant [1]	$\frac{-1}{480}$	$\frac{-1}{1800}$	$\frac{-11}{50400}$	$\frac{-89}{846720}$	$\frac{-5849}{101606400}$
α	90^0	90^0	90^0	89.86^0	89.1^0

Note: P denotes the order of the method while α represents the angle of absolute stability of the methods.

4.0 Numerical Experiment

This section provides experimental results from the TDMM [1],

$$y_{n+1} = y_n + \frac{h}{4}(f_n + 3f_{n+1}) - \frac{h^2}{4} f'_{n+1} + \frac{h^3}{24} f''_{n+1}, \quad p = 4,$$

and the TDHLMM

$$\begin{cases} y_{n+\frac{1}{2}} = \frac{1}{4}(y_n + 3y_{n+1}) - \frac{h}{4} f_{n+1}, & p = 2, \\ y_{n+1} = y_n + \frac{h}{2}(f_n + f_{n+1}) - \frac{h^3}{12} f''_{n+\frac{1}{2}}, & p = 4. \end{cases}$$

on the following initial value problems:

***Problem* 1**: A stiff system of equations

$$\begin{array}{l} y_1' = -8y_1 + 7y_2, \\ y_2' = 42y_1 - 43y_2 \end{array} \quad y(0) = \begin{pmatrix} 1 \\ 8 \end{pmatrix}, \quad x \in [0,1], \quad \begin{cases} y_1(x) = 2e^{-x} - e^{-50x}, \\ y_2(x) = 2e^{-x} + 6e^{-50x}. \end{cases}$$

***Problem* 2**: A stiff system of equations

$$y_1' = -20y_1 - 0.25y_2 - 19.75y_3, \quad y_1(x) = \frac{1}{2}\left(e^{-0.5x} + e^{-20x}(\cos(20x) + \sin(20x))\right),$$

$$y_2' = 20y_1 - 20.25y_2 - 20.25y_3, \quad y_2(x) = \frac{1}{2}\left(e^{-0.5x} - e^{-20x}(\cos(20x) - \sin(20x))\right),$$

$$y_3' = 20y_1 - 19.75y_2 - 20.25y_3, \quad y_1(x) = \frac{1}{2}\left(e^{-0.5x} + e^{-20x}(\cos(20x) - \sin(20x))\right), \quad y(0) = (1 \quad 0 \quad -1)^T, \; x \in [0, 10].$$

To implement (3) on IVPs (1), it is necessary to solve a system of nonlinear algebraic equations for the required solution y_{n+k}. These algebraic equations are solved using a modified form of Newton method

$$y_{n+k}^{[s+1]} = y_{n+k}^{[s]} - (F'(y_{n+k}^{[s]}))^{-1} F(y_{n+k}^{[s]}), \quad s = 0, 1, \ldots$$

where $F'(y_{n+k}^{[s]})$ is the Jacobian matrix of the output method in (3), a function of the vector of ODE systems (1). The starting value $y_{n+1}^{[0]}$ for the Newton scheme is obtained from the explicit one-step formula,

$$y_{n+1}^{[0]} = y_n + \frac{h}{2}(f_{n-1} + f_n).$$

The hybrid LMM is implemented in variable step-size techniques. The starting step-size is $h = 0.01$. The local error estimate at each step is $\left\| y_{n+1}^e - y_{n+1} \right\|$. Suppose we seek to keep $\left\| y_{n+1}^e - y_{n+1} \right\| \le \varepsilon$, then, either upon completion of a successful step or upon failure of a step, we can use

$$h_{new} = 0.9 \times \left(\frac{\varepsilon}{\left\| y_{n+1}^e - y_{n+1} \right\|} \right)^{\frac{1}{p+1}} \times h_{old} \qquad (8)$$

to calculate a new step-size for re-integration or to advance integration. The*p*, 0.9 and ε denotes the order of the TDHLMM, the safety factor and tolerance respectively. In (8), h_{old} is the previous step-size adopted in the last attempt either a successful or a failed step. The alternative approximation formula y_{n+1}^e in (8) is

$$\begin{cases} y_{n+\frac{1}{2}} = \frac{1}{8}\left(y_n + 7y_{n+1}\right) - \frac{3h}{8} f_{n+1} + \frac{h^2}{16} f_{n+1}^{/}, \quad p = 3, \\ y_{n+1}^{e} = y_n + \frac{h}{20}\left(3f_n + f_{n+1}\right) + \frac{4h}{5} f_{n+\frac{1}{2}} + \frac{h^2}{20} f_{n+1}^{/} - \frac{h^3}{120} f_{n+1}^{//}, \quad p = 5, \end{cases}$$

while, y_{n+1} in (8)represents the output point of the TDMM [1] and TDHLMM respectively.

The notations used in the tables are:

ε: Tolerance,

FC: Total number of function calls,

FS: Total number of failed steps,

TS: Total number of steps taken.

Find in Tables 4, 5the numerical results of our experiments.

Table 4: Error in TDHLMM vs TDMM on Problem 1 for comparison

Method	ε	$\left\Vert y_{n+1}^{e} - y_{n+1}\right\Vert$	*FC*	*FS*	*TS*
TDHLMM	10^{-2}	4.5449e-02	75	4	25
TDMM [1]	10^{-2}	5.7000e-03	4036	9	1009
TDHLMM	10^{-4}	1.0429e-04	129	4	43
TDMM [1]	10^{-4}	5.9026e-05	394324	13	98581
TDHLMM	10^{-6}	1.3024e-06	318	3	106
TDMM [1]	10^{-6}	5.9039e-07	684196	15	171048
TDHLMM	10^{-8}	5.7440e-09	942	2	314
TDMM [1]	10^{-8}	5.9042e-09	959508	16	239877
TDHLMM	10^{-10}	5.8524e-11	2889	2	963
TDMM [1]	10^{-10}	5.9048e-11	10397404	17	499351

In Table 4, the local error estimateoftheTDHLMM compares with the TDMM [1] for tolerance 10^{-2} and 10^{-4} respectively but smaller than of the TDMM [1] for the different tolerances 10^{-6}, 10^{-8} and 10^{-10} respectively. The total number of functional calls and the total number of step taking by the hybrid LMM to generate the final output is quite small than that of the TDMM [1]. This serves as advantages of TDHLMM over TDMM [1].

Table 5: Error in TDHLMM vs TDMM on Problem 2 for comparison

Method	*TOL*	$\left\Vert y_{n+1}^{e} - y_{n+1}\right\Vert$	*FC*	*FS*	*TS*
TDHLMM	10^{-2}	5.0621e-02	78	14	26
TDMM [1]	10^{-2}	5.3307e-03	952	10	238
TDHLMM	10^{-4}	2.0439e-05	240	42	80
TDMM [1]	10^{-4}	5.8976e-05	87604	14	21901
TDHLMM	10^{-6}	1.2633e-07	1698	418	566
TDMM [1]	10^{-6}	5.9048e-07	823920	16	205980

Again, in Table 5, the computational cost and the error for the TDHLMM and TDMM [1] respectively for different tolerance shows that the TDHLMM perform better than the TDMM [1] on problem 2 when compared. Judging from the data in Tables 4, 5 it shows that the TDMM [1] are more time consuming owing to the higher number of function evaluations.

5.0 Conclusion

In this paper, we developed a class of $A(\alpha)$-stable third derivative hybrid LMM with variable step-size implementation for the numerical solution of stiff IVPs in ODEs. The order of the TDHLMM shows that the new schemes overcome the Dahlquist order barrier for LMM. Again, the error constants of the TDHLMM are the smaller than that of the TDMM [1] and this serves as an advantage over the TDMM [1].Numerical result shows that the TDHLMM is capable of handling stiff problems.

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