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THIRD DERIVATIVE MULTISTEP METHODS WITH OPTIMIZED REGIONS OF ABSOLUTE STABILITY FOR STIFF IVPS IN ODES

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ABSTRACT

Adam's type methods are known to be zero-stable by design. The backward differentiation formulas are viewed as the dual of the Adams method because of the structure of their second and third characteristics polynomials. Although they are plagued by zero-instability for large step sizes, they are good integrator for stiff initial value problems in ordinary differential equations. This paper is on the derivation of method which combines the characteristics of Adam's type methods and the backward differentiation formulas using the methods of collocation and interpolation. Proposed method is A-stable for order p≤7 and A(α)-stable for p≤12. Numerical examples are presented to show the suitability of method developed in the integration of stiff initial value problems.

1. INTRODUCTION

Consider the initial value problems (IVPs) in ordinary differential equation (ODE) of the form:

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

on the finite interval $I = [x_0, x_N]$ where $y : [x_0, x_N] \to \Re^m$ and $f : [x_0, x_N] X \Re^m \to \Re^m$ where *f* is continuous and twice differentiable, which often aid the formation of Mathematical models of real life phenomena.Solution to Equation (1) is often times insoluble using analytical means, hence the need for numerical techniques in solving such problems.

The numerical methods for solving IVPs in ODEs like Equation (1) are classified into one-step (multistage) methods and multistep (one stage) methods (Hairer and Wanner, 2002), The Runge-Kutta methods belong to the former group, while Adams-Bashforth and Adams-Moulton methods are members of the later (Hairer and Wanner, 2002).

Multiderivative methods for solving systems of ODEs proposed in Enright (1974) and Cash (1981) incorporate higher derivative into their formula. The justification for including higher derivative term into methods is in Enright (1974) and this includes to obtain stability at infinity with reasonable wide stability region in neighborhood of the origin. In Enright (1974), a second derivative linear multistep method was constructed, and this method is of order $p = k+2$ for a k-step.

In this paper, a class of third derivative implicit Adam's type Multistep methods for solving stiff IVPs in ODEs is developed.

2. THIRD DERIVATIVE LINEAR MULTISTEP METHODS (TDLMMs)

The general Third Derivative Linear Multistep Methods (TDLMMs) is of the form:

$$\sum_{j=0}^{k}\alpha_j y_{n+j} = h\sum_{j=0}^{k}\beta_j f_{n+j} + h^2\sum_{j=0}^{k}\gamma_j g_{n+j} + h^3\sum_{j=0}^{k}\delta_j l_{n+j} \tag{2}$$

where α_j, β_j, γ_j, δ_j are real parameters to be determined. If any or all of the parameters β_k, γ_k and δ_k are non-zero, the TDLMMs in (Equation 2) is said to be implicit, else it is explicit. The first, second, third and fourth characteristics polynomials associated with TDLMM in (Equation 2) are given as:

$$\rho(\zeta) = \sum_{j=0}^{k}\alpha_j\zeta^j;\ \sigma(\zeta) = \sum_{j=0}^{k}\beta_j\zeta^j;\ \eta(\zeta) = \sum_{j=0}^{k}\gamma_j\zeta^j;\ \pi(\zeta) = \sum_{j=0}^{k}\delta_j\zeta^j. \tag{3}$$

The order conditions for TDLMM in (Equation 2) is:

$$C_q = \frac{1}{q!}\sum_{j=0}^{k}\left[j^q\alpha_j - qj^{q-1}\beta_j - q(q-1)j^{q-2}\gamma_j - q(q-1)(q-2)j^{q-3}\gamma_j \right],\ q = 0,1,2,\ldots,p \tag{4}$$

The TDLMM in (Equation 2) is of order p, if $C_q = 0$ for $0 \le q \le p$ and $C_{p+1} \neq 0$ is the principal error constant. In Ezzeddinne and Hojjati, (2012), a family of Third derivative multistep methods (TDMM) of the form in Equation 5 was considered and the method was stable for order $p \le 11$ and unstable otherwise. It was designed to bypass stability constraints imposed by the Dahlquist's order barrier theorem (Dahlquist, 1963).

$$y_{n+k} - y_{n+k-1} = h\sum_{j=0}^{k}\alpha_j f_{n+j} + h^2\beta_k g_{n+k} + h^3\gamma_k l_{n+k} \tag{5}$$

The method in Equation (5) has same first, second and third characteristics polynomial with those developed in (Hairer and Wanner, 2002). In situation where methods with high order of accuracy are required, higher derivative methods have been proven to be search direction for the development of high order numerical method for integrating IVPs in (Equation 1). The third derivative multistep methods in Ezzeddinne and Hojjati (2012) are however inefficient in situations for which methods with order as high as p =12 is required. To derive a more efficient method compared to Equation (5) in terms of order of accuracy, a non-zero coefficient will be inputted into the third characteristics polynomial of TDMM in Equation (5). This idea was utilized in Muka and Obiorah (2016) to improve the efficiency of the second derivative backward differentiation formula (SDBDF). The term is introduced in such a way that k-coefficients previously set to zero in the construction of TDMM in Equation (5) is assumed non-zero, and this results in the development of a linear multistep method for each k-step method. Herein, a third derivative linear multistep method of the form in Equation 6 is proposed.

$$y_{n+k} - y_{n+k-1} = h\sum_{j=0}^{k}\beta_j f_{n+k} + h^2\left(\gamma_k g_{n+k} + \gamma_{k-\mu} g_{n+k-\mu}\right) + h^3\delta_k l_{n+k} \tag{6}$$

The term $\gamma_{k-\mu}g_{n+k-k}$ added to Equation (5) leads to the increasing order of method in Equation (6) by one compared with that of TDMM in Equation (5), where the term $\gamma_{k-\mu}$, $\mu=1,2,\ldots,k$ for each μ value is assumed non-zero. The parameters $\delta_k, \gamma_k, \gamma_{k-\mu}$, $\mu=1(1)k$ and β_j, $j=0(1)k$ are real constants to be determined.

3. CONSTRUCTION OF THE METHOD

The collocation and the interpolation methods were used in the construction of the new third derivative multistep method in Equation (6) as follows: Given the power series polynomial, a basic function to approximate the solution of the IVPs in Equation (1).

$$y(x) = \sum_{j=0}^{N} a_j x^j \tag{7}$$

where a_j are the unknown coefficients and $x^j$are the polynomial function, $N=k+4$ is the degree of the polynomial. Differentiating Equation (7) with respect to x results in:

$$y'(x) = f = \sum_{j=1}^{k+4} j a_j x^{j-1} \tag{8}$$

$$y''(x) = f' = g = \sum_{j=2}^{k+4} j(j-1) a_j x^{j-2} \tag{9}$$

$$y'''(x) = f'' = g' = l = \sum_{j=3}^{k+4} j(j-1)(j-2) a_j x^{j-3}\,. \tag{10}$$

Interpolating Equation (7) at $x = x_n$, $x = x_{n+1}$ and collocating Equation (8), Equation (9) and Equation (10) at $x = x_{n+j}$, $j = 1, 2, \ldots, \mathrm{k}$, $x = x_{n+k}$, $x = x_{n+k-\mu}$ and $x = x_{n+k}$ respectively results in the system of linear equations:

$$\begin{pmatrix} 1 & x_{n+k-1} & x_{n+k-1}^2 & x_{n+k-1}^3 & x_{n+k-1}^4 & \cdots & x_{n+k-1}^{k+4} \\ 0 & 1 & 2x_n & 3x_n^2 & 4x_n^3 & \cdots & (k+4)x_n^{k+3} \\ 0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & 4x_{n+1}^3 & \cdots & (k+4)x_{n+1}^{k+3} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 1 & 2x_{n+k} & 3x_{n+k}^2 & 4x_{n+k}^3 & \cdots & (k+4)x_{n+k}^{k+3} \\ 0 & 0 & 2 & 6x_{n+k} & 12x_{n+k}^2 & \cdots & (k+4)(\mathrm{k}+3)x_{n+k}^{k+2} \\ 0 & 0 & 2 & 6x_{n+k-\mu} & 12x_{n+k-\mu}^2 & \cdots & (k+4)(\mathrm{k}+3)x_{n+k-\mu}^{k+2} \\ 0 & 0 & 0 & 6 & 24x_{n+k} & \cdots & (k+4)(\mathrm{k}+3)(\mathrm{k}+2)x_{n+k}^{k+1} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_{k+1} \\ a_{k+2} \\ a_{k+3} \\ a_{k+3} \end{pmatrix} = \begin{pmatrix} y_{n+k-1} \\ f_n \\ f_{n+1} \\ \vdots \\ f_{n+k} \\ g_{n+k} \\ g_{n+k-\mu} \\ l_{n+k} \end{pmatrix} \tag{11}$$

To determine the values of the a_j's, the system in Equation (11) was solved using the Gaussian elimination method, and afterwards the a_j's was substituted into Equation (7) with $x=x_{n+t}$, $\alpha_k=1$ to yield a continuous linear multistep formulas. The resulting scheme was then evaluated at given values of t to obtain the discrete coefficients for fixed k. For each k, we select the $\mu$with the largest α-value and in circumstances where the α-values are the same the one with the smallest error constant is selected as the optimal region of absolute stability. The coefficients of the proposed method in Equation (6) are presented in appendix.

4. STABILITY ANALYSIS

The stability behavior of the new method is examine by applying Equation (6) to the scalar test equation in Equation (12) to give Equation (13) a polynomial of degree three in z.

$$y' = \lambda y, \quad \lambda\ C^{-} \tag{12}$$

$$\zeta^k = \left(1 - z\beta_k - z^2\gamma_k - z^3\delta_k\right)^{-1}\left[\left(1 - z\beta_{k-1}\right)\zeta^{k-1} - z\sum_{j=2}^{k-2}\beta_j\zeta^j - z^2\gamma_{k-\mu}\zeta^{k-\mu}\right] \tag{13}$$

where $z = \lambda h$. If we set $\xi = e^{2\pi i\theta},\ 0 \le \theta < 1$in Equation (13), using the boundary locus method, the roots of the polynomial in Equation (13) describe the stability region R_A of the proposed method in Equation (6). In examining the stability properties of the proposed method in Equation (6), the boundary locus method was used to obtain the boundary describe for each step k. The proposed method in Equation (6) was found to be A-stable for $k \leq 3$ for all values of μ and $A(\alpha)$-stable for k=3,4,…, 8 for all μ and unstable for k>8. The angle of absolute stability including the order and error constants of the proposed TDLMM in Equation (6) and that of TDLMM constructed in (Ezzeddinne and Hojjati, 2012), Equation (5) are presented in Tables 1 and 2 respectively. In Table 1, the stability characteristics of method proposed in this paper are presented, while in Table 2 is the characteristics of the TDMMs of (Ezzeddinne and Hojjati, 2012). The proposed methods in Equation (6) are of higher order with smaller error constants when compared with TDMMs in Equation (5). Both methods are A-stable for stepsizes k=1,2,3. Also, proposed method in Equation (6) has a wider stability region R_A compared with TDMMs in Equation (5).

Table 1: Optimized stability characteristics, order and error constants of Equation (6)

k	1	2	3	4	5	6	7	8
μ	1	1	1	4	5	6	7	8
p	5	6	7	8	9	10	11	12
α	90°	90°	90°	89.9°	88°	81°	78°	75.5°
C_{p+1}	$\frac{1}{7200}$	$\frac{1}{30240}$	$\frac{1}{86400}$	$\frac{2257}{50803200}$	$\frac{3209}{114307200}$	$\frac{267259}{14370048000}$	$\frac{2027801}{158070528000}$	$\frac{1755653}{191792240640}$

Table 2: Stability characteristics, order and error constants of TDMMs in Equation (5)

k	1	2	3	4	5	6	7	8
μ	1	1	1	4	5	6	7	8
p	4	5	6	7	8	9	10	11
α	90°	90°	90°	89.9°	89.1°	77°	77°	65°
C_{p+1}	$\frac{1}{480}$	$\frac{1}{1800}$	$\frac{11}{50400}$	$\frac{89}{846720}$	$\frac{5849}{101606400}$	$\frac{1501}{43545600}$	$\frac{5657}{256608000}$	$\frac{781531}{52690176000}$

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5. NUMERICAL EXPERIMENTS

In this section, the first member of the proposed TDMM in Equation (6) is applied on three standard stiff initial value problems to illustrate the suitability of the proposed methods in the integration of stiff and non-stiff IVPs. The results obtain were compared with the analytic solution of the problems. The starting value for the method was obtained using the second derivative explicit one-step method.,

$$y_{n+1} = y_n + hf_n + \tfrac{1}{2}h^2 f_n' \qquad (14)$$

The following standard problems are considered for the numerical experiments:

Problem 1. Source: Kaps (1981)
Consider the non-linear system of IVPs

$$y_1' = -\left(\varepsilon^{-1} + 2\right) y_1 + \varepsilon^{-1} y_2;\ y_1(0) = 1$$

$$y_2' = y_1 - y_2^2\ ;\ y_2(0) = 1\ ,\ h = 0.001$$

For ε=2. Exact solution is given by: $y_1 = e^{-2t},\quad y_2 = e^{-t}$

Table 3: Numerical solution of problem (1) generated by third derivative method in Equation (6)

t	y_i	TDLMM (6)	Exact	Error $\lvert Y(x)-y_n \rvert$
0.04	y_1	9.234928e-01	9.231163e-01	3.764867e-04
	y_2	9.607941e-01	9.607894e-01	4.692942e-06
0.4	y_1	4.688287e-01	4.493290e-01	1.949976e-03
	y_2	6.727551e-01	6.703200e-01	2.435062e-03

Problem 2: Source : Detest class A_2
Consider the nonlinear problem

$$y' = -\frac{y'}{2},\ y(0) = 1\ ,\ t \in [0,4]\ ,\ h = 0.25$$

Exact solution $y = \dfrac{1}{\sqrt{t+1}}$

Table 4: Numerical solution, problem (2) generated by proposed method in Equation (6)

t	TDLMM (6) y_n	Exact $Y(t_n)$	Error $\lvert Y(t_n)-y_n \rvert$
0.25	8.953325e-01	8.944272e-01	9.053374e-04
2.5	2.078391e-03	5.345225e-01	2.078391e-03
25	1.975199e-01	1.961161e-01	1.403758e-03

Problem 3: (CF: Okuonghae and Nwokorie, 2014)
Consider the linear system of stiff IVP

$$y_1' = -8y_1 + 7y_2,\ y(0) = 1$$

$$y_2' = 42y_1 - 43y_2,\ y(0) = 8$$

$x \in [0,10]$, Exact solution is $\begin{cases} y_1(x) = 2e^{-x} - e^{-50x}, \\ y_2(x) = 2e^{-x} + 6e^{-50x} \end{cases}$, $h = 0.001$

Table 5: Numerical solution, problem (3) generated by proposed method in Equation (6)

t	y_i	TDLMM (6) y_n	Exact $Y(t_n)$	Error $\lvert Y(t_n)-y_n \rvert$
0.04	y_1	1.786108	1.7862436	1.359291e-04
	y_2	2.734417	2.7335906	8.263344e-04
0.4	y_1	1.340651	1.3406401	1.072404e-05
	y_2	1.340651	1.3406401	1.072420e-05
4	y_1	3.663421e-02	3.663128e-02	2.930322e-06
	y_2	3.663421e-02	3.663128e-02	2.930322e-06

6. CONCLUSION

A new class TDLMM is derived by the addition of non-zero term in the third characteristics polynomial of the third derivative multistep methods (TDMMs) derived in (Ezziddenne and Hojjati, 2012). The boundary locus method is used to select stable TDLMM with the largest region of absolute stability. Methods proposed herein is of order one higher than that of TDMMs developed in (Ezziddenne and Hojjati, 2012). This class of method combines the excellent properties of Adam's type method and TDBDF of being zero-stable by design and stable at infinity respectively. TDMMs in Equation (5) is unstable for order $p \leq 11$, but methods proposed in this paper is stable for order upto $p \leq 12$.

7. CONFLICT OF INTEREST

There is no conflict of interest associated with this work.

SUPPLEMENTARY INFORMATION

Table S1: Coefficients of k-step of the proposed TDMM in Equation (6) for each μ. This material is available free of charge via the Internet at http://rjees.com.

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