ON TWO NON-ZERO ROOTS OF MODIFIED SECOND DERIVATIVE BACKWARD DIFFERENTIATION FORMULA (SDBDF) FOR STIFF SYSTEMS



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ABSTRACT

In this paper, an efficient class of second derivative linear multistep method is proposed. The proposed method allows for two non-zero roots of the second characteristics polynomial within the unit circle. The stability of the proposed method is presented and stability regions for certain choices of pair non-zero roots are examined. The method is A-stable for order $p \le 4$ and $A(\alpha)$ -stable for order $p \le 12$. Numerical tests are carried out for suitable comparisons of the proposed method with a well-known subclass of the second derivative linear multistep method.

INTRODUCTION

Suitable methods for the numerical integration of stiff initial value problems are required to satisfy a restrictive condition of A-stability, Cash, (2000). This condition limits attainable order an A-stable Linear Multistep Method (LMM) can achieve. (Athe and Muka, 2017, Butcher, 2008). Researches have scale up the attainable order of methods for integrating stiff initial value problems. Some ways by which this can be done is by the development of methods that allows future points or stages and the use of higher derivatives of solution component incorporated into the method, Athe and Muka (2017), Chakravarti, and Kamel, (1982). The Backward Differentiation Formula (BDF) and its variants are well known for solving stiff initial value problems as it affords an easy means of implementation with a relatively minimum amount of computational effort, Ismail and Ibrahim, (1999). The construction of the second derivative linear multistep method is of importance in this paper as the second derivatives are easily obtainable since continuity and twice differentiability of function of the problem can be guaranteed at all times. Examples of second derivative methods can be found in Hojjati, et. al, (2006), Muka and Obiorah, (2016), Muka and Olu-Oseh, (2017). The success achieved in the Second Derivative Backward Differentiation Formula (SDBDF) is of considerable commendation and as such, research in this direction is unending. The model stiff system is given as

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0, f: R \times R^N \to R^N, y_0 \in R^N$$
 (1)

This paper is on finding efficient second derivative linear multistep methods with better stability characteristics in comparison to the conventional SDBDF.

SECOND DERIVATIVE MULTISTEP METHODS

The general *k*-step Second Derivative Linear Multistep Method (SDLMM) for solving the IVP (1) is of the form

$$\sum_{j=0}^{k} \alpha_{j} y_{n+j} = h \sum_{j=0}^{k} \beta_{j} f_{n+j} + h^{2} \sum_{j=0}^{k} \gamma_{j} f'_{n+j}$$
(2)

where $\alpha_k = 1$, $f'_{n+j} = \frac{df(\mathbf{x}, \mathbf{y}(\mathbf{x}))}{dx} \bigg|_{\mathbf{x} = \mathbf{x}_{n+j}}$, α_j, β_j , and $\gamma_j, j = 0, 1, ..., k$ are parameters to be

determined. The SDLMM (2) is explicit if both β_k or γ_k are zero, else it is implicit. The polynomial notation of the SDLMM (2) is given as

$$\rho(E)y_n = h\sigma(E)f_n + h^2\pi(E)f_n'$$
(3)

where
$$\rho(E) = \sum_{j=0}^{k} \alpha_j E^j$$
, $\sigma(E) = \sum_{j=0}^{k} \beta_j E^j$, and $\pi(E) = \sum_{j=0}^{k} \gamma_j E^j$. (4)

The polynomials: $\rho(E)$; $\sigma(E)$; and $\pi(E)$ are called the first, second and third characteristics polynomials respectively. Taylor series expansion of SDLMM (2) about x_n shows that the SDLMM (2) is of order p, if and only if

$$\sum_{i=0}^{k} \alpha_{j} j^{q} = q \sum_{i=0}^{k} \beta_{j} j^{q-1} + q(q-1) \sum_{i=0}^{k} \gamma_{j} j^{q-2}$$
 (5)

with $0 \le q \le p$.

The error constant of SDLMM (2) is given by

$$C_{p+1} = \sum_{j=0}^{k} \left(\frac{j^{p+1}}{(p+1)!} \alpha_j - \frac{j^p}{p!} \beta_j - \frac{j^{p-1}}{(p-1)!} \gamma_j \right) \neq 0$$
 (6)

Examples of second derivative linear multistep methods are:

i) The Second Derivative Multistep Method (SDMM) (7) in Ismail and Ibrahim, (1999) given as

$$y_{n+1} = y_n + h \sum_{i=0}^{k} \beta_i f_{n+j-k+1} + h^2 \gamma_k f'_{n+1}$$
 (7)

and ii) SDBDF (8) in Ezzeddine and Hojjati (2011) given as

$$y_{n+k} = \sum_{j=0}^{k-1} \alpha_j y_{n+j} + h \beta_k f_{n+k} + h^2 \gamma_k f'_{n+k}$$
 (8)

The k-step SDMM (7) has order of k+2. SDMM (7) is A-stable for k=1,2 and $A(\alpha)$ -stable for $k=3,4,\ldots,7$ and unstable for $k\geq 8$. The SDBDF (8) is a class of k-step formulas having order of k+1. SDBDF (8) is A-stable for k=1,2,3 and $A(\alpha)$ -stable for $k=4,5,\ldots,10$ and unstable for $k\geq 11$.

Considering the third characteristics polynomial of the SDMM (7), notice that all its roots are located at the origin. The idea however is to ensure stability at infinity, Enright, (1974) and Hairer, *et. al*, (2002). However, Chakravarti and Kamel (1982) stated that stability at infinity will still be ensured if all its roots are located within the unit circle. The method derived via the modification of the SDMM (7) for cases of one, two, and three roots not at the origin but within the unit circle yielded SDLMM with an order as high as p = 13. The case of the SDMM (7) having two non-zero roots is given as

$$y_{n+1} = y_n + h \sum_{j=0}^{k} \beta_j f_{n+j-k+1} + h^2 \gamma_k (f'_{n+1} + (a+b)f'_n + abf'_{n-1})$$
 (9)

The stability characteristics of the SDBDF (8) and the SDLMM (9) are given in Tables 1 and 2 respectively

CONSTRUCTION OF METHOD

Consider the second derivative linear multistep method (SDLMM) of the form

$$\sum_{i=0}^{k} \alpha_{j} y_{n+j} = h \beta_{k} (f_{n+k} + (a+b) f_{n+k-1} + ab f_{n+k-2}) + h^{2} \gamma_{k} f'_{n+k}$$
 (10)

where α_j , β_k , and γ_k , are parameters to be determined, a and b are non-zero roots that are less than one in absolute value. If a = b = 0 in (10), reduces to SDBDF. The structure of the polynomials in (10) where |a| < 1, |b| < 1 holds are given as

$$\rho(t) = \sum_{i=0}^{k} \alpha_{j} t^{j}; \quad \sigma(t) = \beta_{k} t^{k-2} (t+a)(t+b), \quad \pi(t) = \gamma_{k} t^{k}$$
 (11)

The linear difference operator associated with the SDLMM (10) is given in (12)

$$L[y(x_n);h] = \sum_{j=0}^{\kappa} [\alpha_j y(x_n + jh)] - h\beta_k (y'(x_n + kh) + (a+b)y'(x_n + (k-1)h) + aby'(x_n + (k-2)h)) - h^2 \gamma_k y''(x_n + kh)$$
(12)

It is assumed here that $y(x_n + jh)$ is differentiable as many times as desired. The other conditions obtained upon Taylor expanding the linear difference operator associated with the SDLMM (10) are given as

$$L[y(x_n); h] = C_0 y(x_n) + C_1 h y'(x_n) + C_2 h^2 y''(x_n) + \dots + C_n h^q y^q(x_n) + \dots$$
 (13)

where

$$C_{0} = \sum_{j=0}^{k} \alpha_{j}$$

$$C_{1} = \sum_{j=0}^{k} j\alpha_{j} - (1 + (a+b) + ab)\beta_{k}$$

$$C_{2} = \sum_{j=0}^{k} \frac{j^{2}}{2!}\alpha_{j} - \beta_{k}(k + (a+b)(k-1) + (ab)(k-2)) - \gamma_{k}$$

$$\vdots$$

$$C_{q} = \sum_{j=0}^{k} \frac{j^{q}}{q!}\alpha_{j} - \frac{\beta_{k}}{(q-1)!}(k^{q-1} + (a+b)(k-1)^{q-1} + ab(k-2)^{q-1}) - \frac{k^{q-2}}{(q-2)!}\gamma_{k}, \quad q = 3, 4, \cdots$$
(14)

The parameters α_j , β_k , and γ_k , are obtained by setting the first (k+2) equations to zero and solving the corresponding linear systems. These parameters are dependent on the non-zero roots a and b. The SDLMM (10) is a class of k-step methods having order p=k+1. The coefficients of the SDLMM (10) are presented in Table 3.

Table 1: Stability characteristics of SDBDF

k	1	2	3	4	5	6	7	8	9	10
p	2	3	4	5	6	7	8	9	10	11
α	90°	90°	90°	89.36°	86.35°	80.82°	72.53°	60.71°	43.39°	12.34°
C_{p+1}	1	1	9	24	600	450	2450	7840	635040 333304301	529200
v_{p+1}	6	21	425	2075	84133	94423	726301	3144919	333304301	353764433

Table 2: Stability characteristics of SDLMM (9)

k	3	4	5	6	7	8	9	10
p	5	6	7	8	9	10	11	12
а	-0.9	-0.9	-0.9	-0.9	-0.5	-0.8	-0.9	-0.8
b	0.2	0.1	-0.1	-0.1	-0.5	-0.3	-0.3	-0.7
α	89.03°	85.32°	80.92°	75.13°	67.76°	56.84°	38.39°	20.2°
c_{p+1}	391	271	507511	723163	579353	452656	376779	557272
P	211200	298620	1023684480	1936478588	2111961600	2145776967	2287832516	4666515293

Table 3: Coefficients of SDLMM (10) for k = 2, 3, ..., 11.

	s: esemeients of BBB	VIIVI (10) 101 R = 2, 3,, 11.	•		
k	2	3	4	5	6
Order	3	4	5	6	7
α_0	1-2(a+b)-11ab	$-\frac{-4+5(a+b)-16ab}{}$	18 - 17(a + b) + 28ab	-144 + 111(a + b) - 124ab	300 - 197(a + b) + 167ab
α_1	$-\frac{F}{2(-4-(a+b)+8ab)}$	$\it G$	$-\frac{5H}{4(32-33(a+b)+72ab)}$	$-\frac{I}{5(225-182(a+b)+228ab)}$	$ \frac{7J}{9(288 - 195(a + b) + 176ab)} $
1	$-\frac{F}{F}$	\overline{G}	5 <i>H</i>		7]
α_2	1	3(-36 + a + b + 32ab)	6(-72 + 93(a + b) + 38ab)	20(200 - 177(a + b) + 294ab)	45(225 - 160(a + b) + 162ab)
		$=\frac{G}{G}$	5 <i>H</i>	I	=
α_3		1	4(-288 + 47(a + b) + 152ab)	10(-900 + 1002(a+b) + 47ab)	20(1200 - 935(a+b) + 1256ab)
			5 <i>H</i>	I	7)
α_4			1	$-\frac{5(-3600 + 857(a + b) + 1284ab)}{1}$	$-\frac{45(900-885(a+b)+109ab)}{}$
α_5				<i>I</i> 1	7J 9(-7200 + 2033(a + b) + 1872ab)
45				·	-
α_6					1
β_{k-2}	$-\frac{6}{F}ab$	$-\frac{66}{G}ab$	$-\frac{120}{H}ab$	$-\frac{8220}{l}ab$	$-\frac{3780}{1}ab$
β_{k-1}	$-\frac{6(a+b)}{}$	$-\frac{66(a+b)}{}$	$-\frac{120(a+b)}{}$	$-\frac{8220}{l}(a+b)$	$-\frac{3780}{1}(a+b)$
	F	\overline{G}	H	1	J
eta_k	$-\frac{6}{-}$	$-\frac{66}{-}$	$-\frac{120}{120}$	$-\frac{8220}{}$	$-\frac{3780}{}$
γ_k	$ \begin{array}{c} F \\ 2 + a + b - 2ab \end{array} $	G $6(3-(a+b)+ab)$	H $12(12-3(a+b)+2ab)$	I = 180(10 - 2(a + b) + ab)	$ \begin{array}{l} J \\ 180(30 - 5(a + b) + 2ab) \end{array} $
- 70	\overline{F}	G	5 <i>H</i>	I	7]
C_{p+1}	4 - 5a - 5b + 16ab	18 - 17a - 17b + 28ab	-144 + 111a + 111b - 124ab	600 - 394a - 394b + 334ab	9(600 - 345b + a(-345 + 236b))
•	84 + 48a + 48b - 60ab	850 + 340a + 340b - 230ab	$\overline{75(-166-51b+3a(-17+8b))}$	84133 + 20958a + 20958b - 7602ab	196(-5781 - 1210b + 2a(-605 + 179b))

where F = -7 - 4a - 4b + 5ab, G = -85 - 34(a + b) + 23ab, H = (-166 - 51(a + b) + 24ab), I = -12019 - 2994(a + b) + 1086ab, J = -5781 - 1210(a + b) + 358ab.

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Table 3: Continuation

where K = -2178903 - 393000a - 393000b + 98330ab, L = -12579676 - 1992445(a + b) + 432290ab

M = -60600782 - 8552740(a + b) + 1639155ab, N = -14618365 - 1859949a(a + b) + 319382ab.

Table 3: Continuation

$$\begin{array}{c} k & 11 \\ \text{Order} & a_0 & \frac{1}{40(226800-89109(a+b)+34564ab)} \\ a_1 & -\frac{77(5488560-2173180(a+b)+853191ab)}{P} \\ a_2 & \frac{275(9486400-3792285(a+b)+1511856ab)}{P} \\ a_3 & -\frac{2475(4002075-1619490(a+b)+658742ab)}{P} \\ a_4 & \frac{3960(6534000-2686775(a+b)+1123332ab)}{P} \\ a_5 & -\frac{97020(508200-213622(a+b)+92951ab)}{P} \\ a_6 & \frac{19404(3659040-1588305(a+b)+736216ab)}{P} \\ a_7 & -\frac{69300(1143450-522505(a+b)+271923ab)}{P} \\ a_8 & \frac{69300(1016400-510955(a+b)+353324ab)}{P} \\ a_9 & -\frac{55(960498000-614697300(a+b)+192335879ab)}{P} \\ a_{11} & \beta_{k-2} & -\frac{11602344600}{P} \\ \beta_{k-1} & -\frac{11602344600}{P} \\ \beta_{k} & -\frac{11602344600}{P} \\ \alpha_{k} & \frac{34927200(55-5(a+b)+ab)}{P} \\ C_{p+1} & -\frac{210(1524600-557155b+a(-557155+195142b))}{13(126a(-18851515+2933193b)-5(4102360483+475058178b))} \\ \text{where } P = -20511802415-2375290890(a+b)+369582318ab. \end{array}$$

STABILITY ANALYSIS

The stability properties of the proposed SDLMM (10) are established. Applying the SDLMM (10) to test equation (15),

$$y'(x) = \lambda y \tag{15}$$

yields the stability polynomial

$$\Pi(t,z) = \sum_{i=0}^{k} \alpha_{j} t^{j} - z \beta_{k} (t^{k} + (a+b)t^{k-1} + (ab)t^{k-2}) - z^{2} \gamma_{k} t^{k}; \quad z = \lambda h$$
(16)

Equating (16) to zero, yields the characteristics equation

$$\Pi(t,z) = \sum_{j=0}^{k} \alpha_j t^j = 0$$
 (17)

Testing for the zero stability of the SDLMM (10), substitute z=0 in (17) and obtain the roots. The k-step SDLMM (10) is zero-stable if the roots t_j , j=1,2,...,k of the first characteristics polynomial $\rho(t)$ are such that $\left|t_j\right| \leq 1$, j=1,2,...,k and $\left|t_j\right| = 1$ being simple.

The roots of the first characteristics polynomial of the SDLMM (10) are dependent on a and b and with only one root equal to unity and other roots can be verified to be less than unity for choices of a and b within the unit circle. Thus, the SDLMM (10) is zero stable. To obtain the region of absolute stability, the boundary locus method is used, Lambert, (1991). Setting $t = e^{i\theta}$, i = 0,1,...,k in (16) yields a polynomial of degree two in z. The roots of $z_j(\theta)$, j = 1,2 describes the stability domain of the SDLMM (10). The search for stable SDLMM (10) is carried out using MATHEMATICA 10 to scan for a and b with the domain (-1,1). The corresponding a-values, and the error constants are presented in Table 4 for certain choices of a, $b \in (-1,1)$.

It is important to note that the comparison of the SDLMM (10) and the SDBDF from Tables 1 and 4, shows that the regions of absolute stability of the SDLMM (10) are larger than those of the SDBDF. There is also a considerable improvement in obtaining stable methods of order 12 of which the SDBDF is unstable for. Table 2 is the stability characteristics of SDLMM (9) with choices of roots a and b within the unit circle.

Table 4.	Stability	characteristics of SDLMM (10)

I dore	1. 50	comity c	iiui uccc	TIBLICE OF		(10)				
k	2	3	4	5	6	7	8	9	10	11
p	3	4	5	6	7	8	9	10	11	12
a	0.6	-0.9	-0.9	-0.9	-0.9	-0.5	-0.8	-0.9	-0.7	-0.4
b	0.2	0.2	0.1	-0.1	-0.1	-0.5	-0.3	-0.3	-0.6	-0.9
α	90°	90°	89.9°	88.2°	83.7°	75.9°	66.6°	53.7°	36.3°	6.27°
c_{p+1}	1	53	1847	8976	108702	18563	153847	2201317	337306	4601
P	60	1393	79600	547739	11120011	2803163	32210026	609602719	118188535	2123557

NUMERICAL TESTS

Numerical experiments are carried out using the SDLMM (10) and the SDBDF (8) to solve three standard DETEST problems in the literature. The Newton-Raphson iterative scheme is used to resolve the implicitness in the methods with a fixed stepsize h. The results are presented in Tables 5-7.

Table 5: Absolute errors of y_1 , y_2 and y_3 solution components for problem 1

Tuon		lessified efforts of y_1, y_2 and y	3 solution components for procient
x	y_i	$ y(x)-y_{SDLMM} $	$ y(x)-y_{SDBDF} $
0.5	y_1	1.22045252E - 6	1.3701995533301273E - 6
	y_2	1.3865571294000012E - 5	1.5528135377002040E - 5
	y_3	1.356077139461398 <i>E</i> - 3	1.5224645626181754E - 3
1.0	y_1	6.408630200196996E - 7	7.3270463502028700E - 7
	y_2	7.404964248995671E - 6	8.4236286829950100E - 6
	y_3	7.120813965624251E - 4	8.1412874672714960E - 4
1.5	y_1	2.941705075304793E - 7	3.5084118752987810 <i>E</i> - 7
	y_2	3.535413577004931E - 6	4.1630323390079440E - 6
	y_3	3.268629723089944E - 4	3.8983106886902874E - 4
2.0	y_1	8.850097234051890E - 8	1.2379229333975283 <i>E</i> – 7
	y_2	1.2350303180003186 <i>E</i> - 6	1.6249915229943346 <i>E</i> — 6
	y_3	9.8338548380816350 <i>E</i> - 5	1.3755153646322071 <i>E</i> - 4

Problem 1

The stiff linear systems

$$y'_1 = -10^4 y_1 + 100 y_2 - 10 y_3 + y_4,$$
 $y_1(0) = 1$
 $y'_2 = -10^3 y_2 + 10 y_3 - y_4,$ $y_2(0) = 1$
 $y'_3 = -y_3 + 10 y_4,$ $y_3(0) = 1$
 $y'_4 = -0.1 y_4,$ $y_4(0) = 1$

 $y_4' = -0.1y_4$, $y_4(0) = 1$ $x \in [0,2]$. Using fixed stepsize of $(h = 10^{-4})$, the absolute errors are shown in Table 5.

In Table 5, the absolute errors of the numerical solutions of the SDLMM (10) and SDBDF (8) are presented. The SDLMM (10) is seen to possess smaller absolute errors when compared with the SDBDF (8).

Problem 2

The Stiff perturbated linear systems

$$y_1' = -2000y_1 + 1000y_2 + 1, \quad y_1(0) = 0$$

 $y_2' = y_1 - y_2, \quad y_2(0) = 0$

 $y_2'=y_1-y_2$, $y_2(0)=0$ $x\in[0,1]$. The absolute errors obtained when solving using a fixed stepsize $(h=10^{-5})$ are presented in Table 6.

Table 6: Absolute errors of y_1 and y_2 solution components for problem 2

1 uc	, ic 0.	Thosofute effors of y ₁ and y ₂	solution components for problem
x	y_i	$ y(x)-y_{SDLMM} $	$ y(x)-y_{SDBDF} $
0.4	y_1	1.0685480099999114E - 7	1.0941540599994446E - 7
	y_2	2.1695454099999317E - 7	2.1877612100000467E - 7
0.6	y_1	9.7984033000059030E - 8	1.0061498399997933E - 7
	y_2	1.9921743799999458 <i>E</i> - 7	2.0117967499999655E - 7
8.0	y_1	8.7111501999976270 <i>E</i> - 8	8.9806106999936260 <i>E</i> - 8
	y_2	1.7747780900001595E - 7	1.7956732000000506E - 7
1.0	y_1	6.9538078999978500E - 8	7.2290280999916070 <i>E</i> - 8
	y_2	1.4233974799998314E - 7	1.4454442500002685E - 7

Problem 3

Consider the linear system

$$y'_1 = -0.5y_1,$$
 $y_1(0) = 1$
 $y'_2 = -y_1,$ $y_2(0) = 1$
 $y'_3 = -100y_3,$ $y_3(0) = 1$
 $y'_4 = -90y_4,$ $y_4(0) = 1$

Consider the linear system $y_1' = -0.5y_1, \quad y_1(0) = 1$ $y_2' = -y_1, \quad y_2(0) = 1$ $y_3' = -100y_3, \quad y_3(0) = 1$ $y_4' = -90y_4, \quad y_4(0) = 1$ $x \in [0,2], \text{ whose exact solution are: } y_1(x) = e^{-0.5x}, y_2(x) = e^{-x}, y_3(x) = e^{-100x}, y_4(x) = e^{-100x}$

The absolute error obtained upon solving problem 1 with SDLMM (10) and SDBDF (8) using fixed stepsize $(h = 10^{-4})$ are displayed in Table 7.

The SDLMM (10) possess smaller absolute errors when compared with the SDBDF (8).

Table 7: Absolute errors of y_1 and y_2 solution components for problem 3

x	y_i	$ y(x)-y_{SDLMM} $	$ y(x)-y_{SDBDF} $
0.5	y_1	1.0795507502692203 <i>E</i> - 4	1.1702832555793297 <i>E</i> - 4
	y_2	1.6614027349903804E - 4	1.8227244692603506E - 4
1.0	y_1	8.4246871762005960E - 5	9.1313126380998530E - 5
	y_2	1.0012175678902890E - 4	1.0990641457703232E - 4
1.5	y_1	6.5793797217994500E - 5	7.1297001847991930 <i>E</i> - 5
	y_2	6.0834443733004395E - 5	6.6769138673983260 <i>E</i> - 5
2.0	y_1	5.0450782865030240E - 5	5.4736682940037530E - 5
	y_2	3.6711909994019410 <i>E</i> - 5	4.0311484430011200 <i>E</i> - 5

The SDLMM (10) possess smaller absolute errors when compared with the SDBDF (8).

CONCLUSION

In this paper, the second characteristics polynomial of the SDBDF (8) is modified so as to accommodate a pair of non-zero roots, this results in a new proposed SDLMM (10). The proposed SDLMM is efficient and possesses a wider region of absolute stability when compared to SDBDF. The integration of three standard problems from DETEST show that absolute errors incurred using the proposed method is smaller when compared with those of SDBDF as shown in Tables 5-7. Therefore, the proposed SDLMM (10) is suitable for the numerical integration of stiff systems.

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