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Modified SDBDF Based on a Non-Zero Root of the Second Characteristics Polynomial

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ABSTRACT

The second derivative backward differentiation formulas (SDBDF) are well known for the integration of stiff initial value problems. In this paper, a class of second derivative linear multistep method (SDLMM) is proposed based on the modification of SDBDF. The proposed class of methods which allows a root of the second characteristics polynomial to be within the unit disc but not at the origin. The class of methods is A-stable for order 4 and $A(\alpha)$-stable up to order $p \leq 11$. Numerical examples are presented to show the application of the proposed methods in the integration of IVPs in ODEs. The results however showed that methods proposed are good integrators in the treatment of stiff problems.

1. Introduction

Numerical methods for the integration of stiff initial value problems (IVPs) (1) are required to be A −Stable. The Dahlquist's second order barrier however constrains A −Stable methods; in that the maximum order of an A −Stable method cannot exceed 2 [1-4].

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

Circumventing the Dahlquist second order barrier constraint has led researchers to develop new methods via direct infusion of higher derivatives of the exact solutions into methods being developed (such methods are known as higher derivative methods [4]). Other research pathways of circumventing the barrier include the addition of new stage or future points. For examples of methods that circumvent the Dahlquist order barrier, see [1, 2, 4-10]. This paper focuses on second derivative linear multistep methods whose stability regions can be fine-tuned using roots of its stability polynomials.

The k-step second derivative linear multistep method (SDLMM) is of the form

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h\sum_{j=0}^{k} \beta_j f_{n+j} + h^2 \sum_{j=0}^{k} \gamma_j f'_{n+j} \tag{2}$$

where $f'_{n+j} \equiv \left.\dfrac{df(x, y(x))}{dx}\right|_{x=x_{n+j}}$, α_j, β_j, and γ_j, are parameters to be determined. The SDLMM (2) can be expressed in compact form as

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

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 $\pi(E)$ in (4) are called the first, second and third characteristics polynomials. The SDLMM (2) is characterized by the polynomials $\rho(E), \sigma(E),$ and $\pi(E)$. The linear difference operator $L[\mathrm{y(x);h}]$ associated with (2) is given by

$$L[\mathrm{y(x}_n\mathrm{);h}] = \sum_{j=0}^{k}[\alpha_j y(x_n+jh) - h\beta_j y'(x_n+jh) - h^2\gamma_j y''(x_n+jh)]. \qquad (5)$$

It is assumed here that y(x) is differentiable as often as we need. Taylor expanding (5) about x_n yields

$$L[\mathrm{y(x}_n\mathrm{);h}] = C_0 y(x_n) + C_1 hy'(x_n) + C_2 h^2 y''(x_n) + \ldots + C_q h^q y^q(x_n) + \ldots \qquad (6)$$

so that

$$\left.\begin{aligned}
C_0 &= \sum_{j=0}^{k}\alpha_j \\
C_1 &= \sum_{j=0}^{k}(j\alpha_j - \beta_j) \\
C_2 &= \sum_{j=0}^{k}\left(\frac{j^2}{2!}\alpha_j - j\beta_j - \gamma_j\right) \\
&\vdots \\
C_q &= \sum_{j=0}^{k}\left(\frac{j^q}{q!}\alpha_j - \frac{j^{q-1}}{(q-1)!}\beta_j - \frac{j^{q-2}}{(q-2)!}\gamma_j\right), \quad q = 3,4,\cdots
\end{aligned}\right\} \qquad (7)$$

The SDLMM (2) and its associated linear difference operator $L[\mathrm{y(x);h}]$ is of order p if $C_0 = C_1 = \ldots = C_p = 0,$ and $C_{p+1} \neq 0.$ $C_{p+1} \neq 0$ is called the error constant. Two prominent sub-classes of SDLMM (2) are second derivative multistep method (SDMM) and second derivative backward differentiation formulas (SDBDF) [4,6]. The first, second and third characteristics polynomials of SDMM and SDBDF are

$$\rho(E) = E^k - E^{k-1};\ \sigma(E) = \sum_{j=0}^{k}\beta_j E^j;\ \pi(E) = \gamma_k E^k \qquad (8)$$

and
$$\rho(E) = \sum_{j=0}^{k}\alpha_j E^j;\ \sigma(E) = \beta_k E^k;\ \pi(E) = \gamma_k E^k \qquad (9)$$

respectively. The roots of first, second and third characteristics polynomials that characterized the SDLMM (2) play critical role in the stability behavior of methods they define.

Definition 1
The $k-$step SDLMM (2) is said to be zero-stable if the roots t_j, $j=1,2,\ldots,k$ of the first characteristics polynomial $\rho(t)$ are such that $|t_j| \leq 1$, $j=1,2,\ldots,k$ and $|t_j|=1$ being simple.

SDMM with first characteristics polynomial in (8) has all its spurious roots at the origin and a root on the boundary of the unit disk. Sub-class of methods with first characteristics polynomial as in (8) are known as Adam's type methods [7], and they are known to be zero stable apriori. SDBDF is zero stable for $k \leq 10$ and unstable otherwise.

Applying SDLMM (2) to the scalar test equation $y'(x)=\lambda y$ gives the stability polynomial

$$\Pi(t,z)=\rho(t)-z\sigma(t)-z^2\pi(t); \quad z=\lambda h \tag{10}$$

Definition 2
The $k-$step SDLMM (2) is said to absolutely stable for a given z, if all the roots of the stability polynomial (10) are such that $|t_j|<1, \quad j=1,2,\dots,k.$

Definition 3
The $k-$step SDLMM (2) is said to have a region of absolute stability R_A, where R_A, is the region of the complex $z-$plane, for that z, for which the method is absolutely stable.

Definition 4
The $k-$step SDLMM (2) is said to be $A-$ stable if its region of absolute stability R_A, contains the entire left of the complex $z-$plane.

The $k-$step SDMM with characteristics polynomial (8) is of order $(\mathrm{k}+2)$, and stable for $k\le 7$ and unstable otherwise. For SDMM, the choice of third characteristics polynomial $\pi(t)$ is made so as to ensure stability at infinity. All the k roots of $\pi(t)$ in (8) are at the origin, Chakravarti and Kamel [11] opined that all the roots are not all required to be at origin, but satisfy the condition $|t_j|<1, \quad j=1,2,\dots,k,$ as this ultimately will not distort the method from being absolutely stable in the left of the complex plane.

The following modifications to the third characteristics polynomial $\pi(t)$ in (8) were proposed in [11], these are:

$$\left.\begin{array}{lll} (i) & \pi(t)=\gamma_k t^k + a\gamma_k t^{k-1}; & |a|<1 \\ (ii) & \pi(t)=\gamma_k t^{k-2}(\mathrm{t}+\mathrm{a})(\mathrm{t}+b); & |a|<1, |b|<1 \\ (iii) & \pi(t)=\gamma_k t^{k-3}(\mathrm{t}+\mathrm{a})(\mathrm{t}+b)(\mathrm{t}+\mathrm{c}); & |a|<1, |b|<1, |c|<1 \end{array}\right\} \tag{11}$$

The numerical test on the influence of the roots $a,b,$ and c on the region of absolute stability show that for (i) $|a|<1$ and $|t_j|=0, \quad j=1,2,\dots,k-1$, then the modified method is stiffly stable for $3\le k\le 8$, (ii) $|a|<1, |b|<1$ and $|t_j|=0, \quad j=1,2,\dots,k-2$, then it is stiffly stable for $3\le k\le 10$, and (iii) $|a|<1, |b|<1, |c|<1$ and $|t_j|=0, \quad j=1,2,\dots,k-3$, then it is stiffly stable for $3\le k\le 12$. By allowing one of the roots of the third characteristics polynomial $\pi(t)$ in (8) to be within the unit circle but not at the origin, stiffly stable method of order 9 is derived. This is an obvious improvement over the SDMM. The SDBDF is $A-$ stable for $k\le 3$ and stiffly stable for $k\le 10$ as shown in Table 1.

Table 1: Stability angles of the 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}	$\frac{1}{6}$	$\frac{1}{21}$	$\frac{9}{425}$	$\frac{24}{2075}$	$\frac{600}{84133}$	$\frac{450}{94423}$	$\frac{2450}{726301}$	$\frac{7840}{3144919}$	$\frac{635040}{333304301}$	$\frac{529200}{353764433}$

Extending the idea of Chakravarti and Kamel in [11] to the SDBDF as to developing higher order SDLMM is the focus of this paper. This paper is organized as follows: section 2 is on the modification of SDBDF, analysis of the stability properties of the modified method is done in section 3. Numerical experiments are presented in section 4 and conclusion is in section 5.

2. Modification of SDBDF

The SDBDF with characteristic polynomials in (9), is modified as

$$\rho(t)=\sum_{j=0}^{k}\alpha_j t^j\,;\ \sigma(t)=\begin{cases}(i)\ \beta_k t^{k-1}(t+a), & |a|<1\\ (ii)\ \beta_k t^{k-2}(t+a)(t+b), & |a|<1,|b|<1\\ (iii)\ \beta_k t^{k-3}(t+a)(t+b)(t+c), & |a|<1,|b|<1,|b|<1\end{cases}\ ;\ \pi(t)=\gamma_k t^k \quad (12)$$

The coefficients of t^j of method with characteristics polynomials (12) are determined using the undetermined and Taylors' series expansion methods. For the case where a root of the second characteristics polynomial $\sigma(t)$ is not at the origin, that is

$$\rho(t)=\sum_{j=0}^{k}\alpha_j t^j\,;\ \sigma(t)=\beta_k t^{k-1}(t+a),\ \ |a|<1;\ \pi(t)=\gamma_k t^k \qquad (13)$$

the order condition for SDLMM (13) can be obtained from (7) as

$$\left.\begin{aligned}C_0 &= \sum_{j=0}^{k}\alpha_j\\ C_1 &= \sum_{j=0}^{k}j\alpha_j-(1+a)\beta_k\\ C_2 &= \sum_{j=0}^{k}\frac{j^2}{2!}\alpha_j-\beta_k(k+a(k-1))-\gamma_k\\ &\vdots\\ C_q &= \sum_{j=0}^{k}\frac{j^q}{q!}\alpha_j-\frac{\beta_k}{(q-1)!}(k^{q-1}+a(k-1)^{q-1})-\frac{k^{q-2}}{(q-2)!}\gamma_k,\quad q=3,4,\cdots\end{aligned}\right\}\qquad (14)$$

For $k=1$ SDLMM (13), we solve $C_0=C_1=C_2=0$ in equation (14). Similarly, for $k=2$, we solve $C_0=C_1=C_2=C_3=0$ The parameters obtained by solving the linear system (14), are dependent on the non-zero root a of the second characteristics polynomial $\sigma(t)$ in (13). In Table 2, are parameters of the SDLMM (13) for $k\geq 3$.

3. Stability Analysis

In this section the stability properties of the SDLMM defined by the characteristics polynomial (13) is investigated with regards to zero-stability and region of absolute stability R_A. Applying the SDLMM (13) to the test equation $y'(x)=\lambda y$, yields the stability polynomial

$$\Pi(t,z)=\sum_{j=0}^{k}\alpha_j t^j-z\beta_k(t^k+at^{k-1})-z^2\gamma_k t^k;\quad z=\lambda h \qquad (15)$$

The parameters $\alpha_j,\ j=0,1,\ldots,k-1$ are functions of the non-zero root a of the second characteristics polynomial $\sigma(t)$ in (13), therefore the roots of the stability polynomial (15) and first characteristic polynomial (16) are dependent on a.

$$\Pi(t,0)=\sum_{j=0}^{k}\alpha_j t^j; \qquad (16)$$

Table 2: Coefficients and Error constants for SDLMM(13) for $k = 3,4,\ldots,10$.

K	3	4	5	6	7	8	9	10
Order	4	5	6	7	8	9	10	11
α_0	$-\frac{4-5a}{17(5+2a)}$	$-\frac{-18+17a}{5(166+51a)}$	$\frac{3(-48+37a)}{12019+2994a}$	$-\frac{-300+197a}{7(5781+1210a)}$	$\frac{90(-40+23a)}{726301+131000a}$	$-\frac{45(-980+503a)}{12579676+1992445a}$	$\frac{35(-2240+1041a)}{30300391+4276370a}$	$-\frac{14(-22680+9649a)}{11(14618365+1859949a)}$
α_1	$-\frac{3(-9+14a)}{17(5+2a)}$	$\frac{4(-32+33a)}{5(166+51a)}$	$-\frac{5(-225+182a)}{12019+2994a}$	$\frac{27(-96+65a)}{7(5781+1210a)}$	$-\frac{14(-2450+1439a)}{726301+131000a}$	$\frac{240(-1920+1001a)}{12579676+1992445a}$	$-\frac{45(-19845+9334a)}{30300391+4276370a}$	$\frac{175(-22400+9621a)}{11(14618365+1859949a)}$
α_2	$\frac{3(-36+a)}{17(5+2a)}$	$-\frac{18(-24+31a)}{5(166+51a)}$	$\frac{20(-200+177a)}{12019+2994a}$	$-\frac{225(-45+32a)}{7(5781+1210a)}$	$\frac{189(-784+475a)}{726301+131000a}$	$-\frac{392(-5600+2983a)}{12579676+1992445a}$	$\frac{240(-19440+9289a)}{30300391+4276370a}$	$-\frac{2025(-11025+4793a)}{11(14618365+1859949a)}$
α_3	1	$\frac{4(-288+47a)}{5(166+51a)}$	$-\frac{60(-150+167a)}{12019+2994a}$	$\frac{100(-240+187a)}{7(5781+1210a)}$	$-\frac{1575(-245+156a)}{726301+131000a}$	$\frac{3528(-1792+985a)}{12579676+1992445a}$	$-\frac{784(-18900+9229a)}{30300391+4276370a}$	$\frac{3600(-21600+9541a)}{11(14618365+1859949a)}$
α_4		1	$\frac{5(-3600+857a)}{12019+2994a}$	$-\frac{675(-60+59a)}{7(5781+1210a)}$	$\frac{350(-1960+1369a)}{726301+131000a}$	$-\frac{7350(-1680+971a)}{12579676+1992445a}$	$\frac{1764(-18144+9145a)}{30300391+4276370a}$	$-\frac{8820(-21000+9481a)}{11(14618365+1859949a)}$
α_5			1	$\frac{9(-7200+2033a)}{7(5781+1210a)}$	$-\frac{1890(-490+433a)}{726301+131000a}$	$\frac{3920(-4480+2843a)}{12579676+1992445a}$	$-\frac{2940(-17010+9019a)}{30300391+4276370a}$	$\frac{15876(-20160+9397a)}{11(14618365+1859949a)}$
α_6				1	$\frac{63(-19600+6067a)}{726301+131000a}$	$-\frac{17640(-1120+901a)}{12579676+1992445a}$	$\frac{3920(-15120+8809a)}{30300391+4276370a}$	$-\frac{22050(-18900+9271a)}{11(14618365+1859949a)}$
α_7					1	$\frac{72(-313600+102363a)}{12579676+1992445a}$	$-\frac{5040(-11340+8389a)}{30300391+4276370a}$	$\frac{25200(-16800+9061a)}{11(14618365+1859949a)}$
α_8						1	$\frac{27(-2116800+712843a)}{30300391+4276370a}$	$-\frac{28350(-12600+8641a)}{11(14618365+1859949a)}$
α_9							1	$\frac{5(-63504000+21769309a)}{11(14618365+1859949a)}$
α_{10}								1
β_{k-1}	$\frac{66}{17(5+2a)}a$	$\frac{120}{166+51a}a$	$\frac{8220}{12019+2994a}a$	$\frac{3780}{5781+1210a}a$	$\frac{457380}{726301+131000a}a$	$\frac{7670880}{12579676+1992445a}a$	$\frac{17965080}{30300391+4276370a}a$	$\frac{8454600}{14618365+1859949a}a$
β_k	$\frac{66}{17(5+2a)}$	$\frac{120}{166+51a}$	$\frac{8220}{12019+2994a}$	$\frac{3780}{5781+1210a}$	$\frac{457380}{726301+131000a}$	$\frac{7670880}{12579676+1992445a}$	$\frac{17965080}{30300391+4276370a}$	$\frac{8454600}{14618365+1859949a}$
γ_k	$\frac{6(-3+a)}{17(5+2a)}$	$\frac{36(-4+a)}{5(166+51a)}$	$\frac{360(-5+a)}{12019+2994a}$	$\frac{900(-6+a)}{7(5781+1210a)}$	$\frac{12600(-7+a)}{726301+131000a}$	$\frac{176400(-8+a)}{12579676+1992445a}$	$\frac{352800(-9+a)}{30300391+4276370a}$	$\frac{1587600(-10+a)}{11(14618365+1859949a)}$
C_{p+1}	$\frac{18-17a}{850+340a}$	$\frac{48-37a}{4150+1275a}$	$\frac{600-394a}{84133+20958a}$	$-\frac{135(-40+23a)}{196(5781+1210a)}$	$\frac{4900-2515a}{1452602+262000a}$	$\frac{31360-14574a}{12579676+1992445a}$	$\frac{635040-270172a}{333304301+47040070a}$	$-\frac{105(-25200+9901a)}{121(14618365+1859949a)}$

A numerical scan for parameters that yield stable SDLMM with characteristics polynomials (13) for value of a within the range $a \in (-1,1)$ is carried out using MATHEMATICA 10. In Table 3, the stability characteristics of zero-stable SDLMM (13) with the widest stability region R_A is presented.

Table 3: Stability characteristics of SDLMM (13)

k	1	2	3	4	5	6	7	8	9	10
a	0.9	0.7	0.8	−0.7	−0.9	−0.9	−0.9	−0.9	−0.9	−0.9
p	2	3	4	5	6	7	8	9	10	11
α	90°	90°	90°	89.97°	88.19°	83.46°	76.28°	65.82°	53.81°	29.2°
c_{p+1}	$-\frac{4}{57}$	$\frac{5}{1176}$	$\frac{1}{255}$	$\frac{739}{32575}$	$\frac{4773}{326354}$	$\frac{5463}{613088}$	$\frac{14327}{2433604}$	$\frac{6968}{1689881}$	$\frac{5332}{1766627}$	$\frac{1462}{639341}$

4. Numerical Experiment

The SDLMM (13) is used to integrate stiff linear and nonlinear problems in this section, results obtained are compared with those generated using the SDBDF (9). To resolve the implicitness in the implementation of the methods, the Newton-Raphson iterative scheme is used [2, 4, 7]. Implementation is done using a fixed step size, h.

Problem 1

Consider the nonlinear system

$$y_1' = -1002y_1 + 1000{y_2}^2, \qquad y_1(0) = 1$$
$$y_2' = y_1 - y_2(1 + y_2), \qquad y_2(0) = 1$$

$x \in [0,5]$, whose exact solutions are: $y_1(x) = e^{-2x}, y_2(x) = e^{-x}$ [12].

The absolute errors obtained upon solving problem 1 with $SDLMM$ (13) and $SDBDF$ using fixed stepsize $h = 10^{-4}$ are displayed in Table 4.

Table 4: Absolute errors of y_1 and $y_2$solution components for problem 1

x	y_i	$\lvert y(x) - y_{SDLMM}\rvert$	$\lvert y(x) - y_{SDBDF}\rvert$
1	y_1	$8.066283250601769E-5$	$8.117704156002103E-5$
	y_2	$1.0894973361402771E-4$	$1.1034758718098114E-4$
2	y_1	$1.091655783900039E-5$	$1.0986148467000134E-5$
	y_2	$4.008048003900644E-5$	$4.0594721627013050E-5$
3	y_1	$1.4773995779997565E-6$	$1.4868176459997134E-6$
	y_2	$1.474482610300254E-5$	$1.4934005010999729E-5$
4	y_1	$1.9994485000004092E-7$	$2.0121944700003452E-7$
	y_2	$5.424333650000390E-6$	$5.4939286810024020E-6$
5	y_1	$2.7059667999997398E-8$	$2.7232165999998660E-8$
	y_2	$1.9955064460000158E-6$	$2.0211090270005894E-6$

From Table 4, it can be observed that the SDLMM (13) tracks the exact solution to at least 4 digits. The SDLMM (13) possesses smaller absolute errors compared to that of the SDBDF.

Problem 2

The stiff linear systems

$$y_1' = 998y_1 + 1998y_2, \qquad y_1(0) = 1$$
$$y_2' = -999y_1 - 1999y_2, \qquad y_2(0) = 0$$

$x \in [0,1]$, whose exact solutions are: $y_1(x) = -e^{-1000x} + 2e^{-x}$, $y_2(x) = e^{-1000x} - e^{-x}$ [12]. Using fixed stepsize of $(h = 10^{-5})$, the absolute errors are shown in Table 5.

Table 5: Absolute errors of y_1 and $y_2$solution components for problem 2

x	y_i	$\lvert y(x) - y_{SDLMM} \rvert$	$\lvert y(x) - y_{SDBDF} \rvert$
0.1	y_1	$4.741271129704572E-5$	$5.428943224194960E-5$
	y_2	$2.3706355648300814E-5$	$2.7144716120530710E-5$
0.2	y_1	$4.290079664270863E-5$	$4.912311106775036E-5$
	y_2	$2.1450398321576358E-5$	$2.456155553387518E-5$
0.4	y_1	$4.047154779307505E-6$	$4.021860395475585E-5$
	y_2	$1.756210189041152E-5$	$2.0109301977377925E-5$
0.6	y_1	$2.8685539941397664E-5$	$3.292820972911059E-5$
	y_2	$1.4378633819256414E-5$	$1.6464104864555296E-5$
0.8	y_1	$2.3544460894142638E-5$	$2.6959339453180853E-5$
	y_2	$1.1772230447015808E-5$	$1.3479669726590426E-5$
1.0	y_1	$1.927657543498995E-5$	$2.2072441529630282E-5$
	y_2	$9.638287717328442E-6$	$1.103622076431554E-5$

The SDLMM (13) possesses smaller absolute errors compared to that of the SDBDF.

Problem 3

The stiff linear systems

$$y_1' = -y_1 + y_2, \qquad y_1(0) = 1$$
$$y_2' = -100y_1 - y_2, \qquad y_2(0) = 0$$
$$y_3' = -100y_3 + y_4, \qquad y_3(0) = 1$$
$$y_4' = -10000y_3 - 100y_4, \qquad y_4(0) = 0$$

whose exact solutions are: $y_1 = e^{-x}\cos 10x$, $y_2 = -10e^{-x}\sin 10x$, $y_3 = e^{-100x}\cos 100x$, $y_4 = -100e^{-100x}\sin 100x$ [12]. Using $(h = 10^{-5})$, the problem is solved at a point $x = 0.1$ and the absolute errors are presented in Table 6.

Table 6: Absolute errors of y_1 and y_4 solution components for problem 3

x	y_i	$\lvert y(x) - y_{SDLMM} \rvert$	$\lvert y(x) - y_{SDBDF} \rvert$
0.1	y_1	$2.430664595641008E-3$	$2.4325204562850034E-3$
	y_4	$2.293631606082000E-3$	$2.2936322928490000E-3$

The absolute errors when SDLMM (13) is used is smaller compared to that of the SDBDF.

5. Conclusion

A new class of second derivative linear multistep method is developed by considering a non-zero root in the second characteristics polynomial $-\sigma(t)$ of the SDBDF (9). Comparing the stability characteristics of the SDLMM (13) and the SDBDF (9) in Tables 1 and 3, the SDLMM (13) was observed to possess a wider region of absolute stability R_A. From the numerical experiments performed, the strength of the SDLMM (13) in tracking the exact solutions is visible. The SDLMM possesses the same order with the SDBDF and compares favourably when used to integrate stiff systems.

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