$L(\alpha)$-Stable Second Derivative Block Multistep Formula for Stiff Initial Value Problems

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Abstract— **A block multistep method is developed from a second derivative continuous multistep scheme with Chebyshev points as collocation points for the integration of stiff initial value problems. The order, stability analysis are investigated and the method is shown to be $L(\alpha)$-stable, which is a requirement for numerical integration of stiff initial value problems. Some experimental problems reveal that the method is suitable for the solution of stiff initial value problems.**

Keywords: ***Continuous Schemes, Multistep Collocation, Chebyshev points, Second Derivative***

1 Introduction

The numerical integration of stiff initial value problems has been the main interest of researchers in numerical analysis. Although there has been various mathematical definition attached to this concept. (see [18]). Given a system of ordinary differential equations of the form

$$y' = Ay + \phi(x), \qquad y(a) = \eta, \qquad a \leq x \leq b \quad (1)$$

where $y = (y_1, y_2, \cdots, y_s)$ and $\eta = (\eta_1, \eta_2, \cdots, \eta_s)$. Let λ_i be the eigenvalues of the $s \times s$ matrix A, (1) is said to be stiff if $Re(\lambda_i) < 0$, $i = 1, 2, \cdots, s$, and $Max\,|Re(\lambda_i)| >> Min\,|Re(\lambda_i)|$.

In [9], the famous theorem of Dahlquist [9] known as the Dahlquist barrier open a new research direction in the development of numerical algorithm for solution of stiff IVPs. This made some researchers [2,29] relax some stability conditions so as to circumvent the Dahlquist barrier. A survey of methods for stiff problems can be found in literatures [14,15].

In what follows, we shall construct a block second derivative block multistep with Chebyshev collocation point, where the nodes are also included in the collocation points as zeros of the shifted Chebyshev polynomials. We shall obtain this block method from a single continuous multistep scheme with power series interpolating polynomial. [10,17,21]

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This article is organized as follows: We give the block formula represented in a block matrix form in section 2. Some characteristics of the method is investigated and analyzed in section 3. Finally we solve some problems to show comparison with some related works.

2 Theoretical Procedure

To solve a stiff initial value problem

$$y' = f(x, y), \qquad y(x_0) = y_0 \qquad (2)$$

on the interval $I = [x_0, x_N]$, where y and f are assumed to be continuously differentiable and satisfy the conditions to guarantee the existence and uniqueness of solution of the initial value problem.

Using a multistep collocation technique, with collocation points $\mathbf{v} = \{k \cdot x : T_k^*(x) = 0\} = \{v_1, v_2, \cdots, v_k\}$ of the roots of a Chebyshev polynomial $(T_k^*(x))$ as the off-grid points in the proposed integration formula, the interpolating function for a 2-step method is given as

$$y(x) = \sum_{j=0}^{5} a_j \left(\frac{x - x_n}{h}\right)^j. \qquad (3)$$

For $k = 2$, we have that $\mathbf{v} = \{2 \cdot x : T_2^*(x) = 0\} = \{1 - \frac{1}{2}\sqrt{2}, 1 + \frac{1}{2}\sqrt{2}\}$. Hence, it is necessary to interpolate (10) at points $x = \{x_n, x_{n+1-\frac{1}{2}\sqrt{2}}, x_{n+1}, x_{n+1+\frac{1}{2}\sqrt{2}}\}$, and collocate $y'(x)$ and $y''(x)$ at $x = x_{n+2}$. We obtain a system of equations represented in the matrix form

$$AB = C \qquad (4)$$

where A=

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & a_{42} & a_{43} & a_{44} & a_{45} & a_{46} \\ 0 & 1 & 4 & 12 & 32 & 80 \\ 0 & 0 & 2 & 12 & 48 & 160 \end{pmatrix}$$

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with

$$a_{22}=1-\frac{1}{2}\sqrt{2}, a_{23}=-\sqrt{2}+\frac{3}{2}, a_{24}=-\frac{7}{4}\sqrt{2}+\frac{5}{2}$$

$$a_{25}=-3\sqrt{2}+\frac{17}{4}, a_{26}=-\frac{41}{8}\sqrt{2}+\frac{29}{4}, a_{42}=1+\frac{1}{2}\sqrt{2}$$

$$a_{43}=\sqrt{2}+\frac{3}{2}, a_{44}=\frac{7}{4}\sqrt{2}+\frac{5}{2}, a_{45}=3\sqrt{2}+\frac{17}{4}$$

$$a_{46}=\frac{41}{8}\sqrt{2}+\frac{29}{4}$$

$$B=[a_0,a_1,a_2,a_3,a_4,a_5]^T$$

$$C=\left[y_n, y_{n+1-\frac{1}{2}\sqrt{2}}, y_{n+1}, y_{n+1+\frac{1}{2}\sqrt{2}}, hf_{n+2}, h^2g_{n+2}\right]^T$$

solving the system of equation (4) for variable $B=[a_0,a_1,a_2,a_3,a_4,a_5]^T$ and substituting in (3), we obtain a continuous multistep formula

$$\begin{aligned} y(x) &= \sum_{j=0}^{1}\alpha_j(x)y_{n+j}+\sum_{j=1}^{2}\alpha_{v_j}(x)y_{n+v_j}+h\beta_2(x)f_{n+2} \\ &= +h^2\delta_2(x)g_{n+2} \end{aligned} \tag{5}$$

where

$$\alpha_0(x) = 1-\frac{172}{29}x+\frac{946}{87}x^2-\frac{755}{87}x^3+\frac{92}{29}x^4-\frac{38}{87}x^5$$

$$\alpha_{v_1}(x) = \begin{pmatrix} \left(\frac{64}{29}\sqrt{2}+\frac{136}{29}\right)x+\left(-\frac{352}{87}\sqrt{2}-\frac{404}{29}\right)x^2 \\ +\left(\frac{422}{29}+\frac{200}{87}\sqrt{2}\right)x^3+\left(-\frac{14}{29}\sqrt{2}-\frac{182}{29}\right)x^4 \\ +\left(\frac{28}{29}+\frac{2}{87}\sqrt{2}\right)x^5 \end{pmatrix}$$

$$\alpha_1(x) = -\frac{100}{29}x+\frac{1478}{87}x^2-\frac{1777}{87}x^3+\frac{272}{29}x^4-\frac{130}{87}$$

$$\alpha_{v_2} = \begin{pmatrix} \left(\frac{136}{29}-\frac{64}{29}\sqrt{2}\right)x+\left(-\frac{404}{29}+\frac{352}{87}\sqrt{2}\right)x^2 \\ +\left(-\frac{200}{87}\sqrt{2}+\frac{422}{29}\right)x^3+\left(\frac{14}{29}\sqrt{2}-\frac{182}{29}\right)x^4 \\ +\left(\frac{28}{29}-\frac{2}{87}\sqrt{2}\right)x^5 \end{pmatrix}$$

$$\beta_2 = -\frac{15}{29}x+\frac{242}{87}x^2-\frac{355}{87}x^3+\frac{64}{29}x^4-\frac{34}{87}x^5$$

$$\delta_2 = \frac{4}{29}x-\frac{131}{174}x+\frac{199}{174}x-\frac{19}{29}x+\frac{11}{87}x^5$$

Evaluating (5) at $x=x_{n+2}$ yields the main method, while differentiating (5) and evaluating at $x=\{x_{n+1-\frac{1}{2}\sqrt{2}}, x_{n+1}, x_{n+1+\frac{1}{2}\sqrt{2}}\}$ together, yields the block method represented in block matrix finite difference form

$$AY_m = BY_{m-1}+hCF_m+h^2DG_m \tag{6}$$

where A=

$$\begin{pmatrix} \left(\frac{38}{87}-\frac{9}{58}\sqrt{2}\right) & \left(\frac{91}{87}\sqrt{2}+\frac{19}{29}\right) & \left(-\frac{26}{87}-\frac{23}{58}\sqrt{2}\right) & 0 \\ \left(-\frac{70}{87}\sqrt{2}+\frac{6}{29}\right) & -\frac{61}{87} & \left(\frac{70}{87}\sqrt{2}+\frac{6}{29}\right) & 0 \\ \left(\frac{23}{58}\sqrt{2}-\frac{26}{87}\right) & \left(\frac{19}{29}-\frac{91}{87}\sqrt{2}\right) & \left(\frac{38}{87}+\frac{9}{58}\sqrt{2}\right) & 0 \\ \left(-\frac{32}{87}\sqrt{2}+\frac{16}{29}\right) & -\frac{8}{87} & \left(\frac{32}{87}\sqrt{2}+\frac{16}{29}\right) & -1 \end{pmatrix},$$

$$B=\begin{pmatrix} 0 & 0 & 0 & \left(\frac{43}{87}\sqrt{2}+\frac{23}{29}\right) \\ 0 & 0 & 0 & -\frac{25}{87} \\ 0 & 0 & 0 & \left(-\frac{43}{87}\sqrt{2}+\frac{23}{29}\right) \\ 0 & 0 & 0 & \frac{1}{87} \end{pmatrix}$$

$$C=\begin{pmatrix} 1 & 0 & 0 & \left(\frac{11}{87}\sqrt{2}-\frac{13}{29}\right) \\ 0 & 1 & 0 & \frac{28}{87} \\ 0 & 0 & 1 & \left(-\frac{11}{87}\sqrt{2}-\frac{13}{29}\right) \\ 0 & 0 & 0 & -\frac{22}{87} \end{pmatrix}$$

$$D=\begin{pmatrix} 0 & 0 & 0 & \left(\frac{5}{58}-\frac{1}{87}\sqrt{2}\right) \\ 0 & 0 & 0 & -\frac{13}{174} \\ 0 & 0 & 0 & \left(\frac{5}{58}+\frac{1}{87}\sqrt{2}\right) \\ 0 & 0 & 0 & -\frac{2}{87} \end{pmatrix}.$$

The 4-dimensional vector Y_m, Y_{m-1}, F_m and G_m have collocation points specified as,

$$\begin{aligned} Y_m &= [y_{n+v_1}, y_{n+1}, y_{n+v_2}, y_{n+2}]^T, \\ Y_{m-1} &= [y_{n-v_2}, y_{n-1}, y_{n-v_1}, y_n]^T, \\ F_m &= [f_{n+v_1}, f_{n+1}, f_{n+v_2}, f_{n+2}]^T, \\ G_m &= [g_{n+v_1}, g_{n+1}, g_{n+v_2}, g_{n+2}]^T. \end{aligned}$$

3 Analysis of the Method

The analysis of the $L(\alpha)$-stable block multistep method is presented in this section. Numerical Properties such as Order and Error constant, consistency, stability and convergence are investigated.

Order and Error Constant

Let the individual linear multistep method with Chebyshev collocation points be associated with the formula

$$L[y(x_n;h)] = \sum_{j=0}^{k} \begin{pmatrix} \overline{\alpha}_j y(x+jh) + \overline{\alpha}_{v_j} y(x+v_jh) \\ -h\overline{\beta}_j y'(x+jh) - h\overline{\beta}_{v_j} y'(x+v_jh) \\ -h^2\overline{\delta}_k y''(x_n+kh) \end{pmatrix} \tag{7}$$

where $y(x)$ is an arbitrary smooth function on $[a,b]$. Expanding (18) with Taylor series expansions of $y(x+jh)$, $y(x+v_jh)$, $y'(x+jh)$, $y'(x+v_jh)$ and $y''(x+kh)$, $j=0,v_1,1,v_2,2,...,v_k,k$ to obtain the expression

$$L[y(x_n;h)] = \overline{C}_0 y(x) + \overline{C}_1 hy'(x) + \cdots + \overline{C}_p h^p y^{(p)}(x) + \cdots$$

where $\overline{C}_i$ are vectors in the form,

$$\overline{C}_0 = \sum_{j=0}^{k} \overline{\alpha}_j + \sum_{j=1}^{k} \overline{\alpha}_{v_j} \tag{8}$$

$$\overline{C}_1 = \sum_{j=0}^{k} j\overline{\alpha}_j + \sum_{j=1}^{k} v_j\overline{\alpha}_{v_j} - \left(\sum_{j=0}^{k}\overline{\beta}_j + \sum_{j=1}^{k}\overline{\beta}_{v_j}\right) \tag{9}$$

$$\overline{C}_2 = \frac{1}{2!}\left(\sum_{j=0}^{k} j^2\overline{\alpha}_j + \sum_{j=1}^{k} v_j^2\overline{\alpha}_{v_j}\right) - \left(\sum_{j=0}^{k} j\overline{\beta}_j + \sum_{j=1}^{k} v_j\overline{\beta}_{v_j}\right) - \overline{\delta}_k \tag{10}$$

$$\cdots$$

$$\overline{C}_q = \frac{1}{q!}\left(\sum_{j=0}^{k} j^q\overline{\alpha}_j + \sum_{j=1}^{k} v_j^q\overline{\alpha}_{v_j}\right) - \frac{1}{(q-1)!}\left(\sum_{j=0}^{k} j^{q-1}\overline{\beta}_j + \sum_{j=1}^{k} v_j^{q-1}\overline{\beta}_{v_j}\right) - \frac{1}{(q-2)!}k^{q-2}\overline{\delta}_k \tag{11}$$

$$q = 0,1,2,\cdots,p.$$

Definition 3.1

The block multistep method with Chebyshev collocation points (6) and the associated linear difference operator is said to be of ***order*** p if,

$$\overline{C}_0 = \overline{C}_1 = \overline{C}_2 = \cdots = \overline{C}_p = \overline{0}, \qquad \overline{C}_{p+1} \neq \overline{0}. \tag{12}$$

Definition 3.2

The term $\overline{C}_{p+1}$ is called the *Error Constant (EC)* and the local truncation error for the method is given by,

$$\overline{t}_{n+k} = \overline{C}_{p+1} h^{p+1} y^{(p+1)} x_n + O(h^{(p+2)}). \tag{13}$$

Using the appropriate coefficients in (6), methods are of order $p = [5,5,5,5]^T$ with error constants $\overline{C}_6 =$

$$\left[-1.38\times10^{-3}, 9.02\times10^{-4}, -4.88\times10^{-4}, -6.39\times10^{-5}\right].^T$$

Consistency

Since the block multistep method is of order $p = 5 \geq 1$, therefore it is consistent. Henrici [16]

Zero Stability of Block Multistep Method

Applying the block multistep method (6) to the test problem

$$y' = \lambda y,$$

with $z = \lambda h$, solving the characteristic equation $det|\xi\cdot(A - Cz - Dz^2) - B| = 0$ for ξ at $z \to 0$, the roots $\{0,0,0,1\}$ of the resulting equation are less than or equal to 1, therefore the numerical method is zero-stable.

Convergence

Since the Block multistep method is consistent and zero-stable, we can safely assert the convergence of the new method. (Henrici [16])

Region of Absolute Stability of new method

Solving characteristic equation

$$det|\xi\cdot(A - Cz - Dz^2) - B| = 0$$

for ξ, we obtain the stability function as

$$R(z) = -\frac{120 + 72z + 15z^2 + z^3}{-120 + 168z - 111z^2 + 45z^3 - 12z^4 + 2z^5} \tag{14}$$

Solving (14), we obtain the stability region $\mathcal{S} = [(-\infty,0)\bigcup(4.11,\infty)]$.

The block multistep method is A_0-Stable and satisfies $A(\alpha)$-Stability with stiff stability properties $\alpha = 89.85°$, $D = 0.066$ and $y = 1.4$. Hence, *The method is Stiffly Stable.* The region of absolute stability is presented in Figure 2.

Test for L(α)-Stability

The numerical method is A(α)-stable and $\lim_{z\to-\infty} R(z) = 0$, we say that block multistep method is L(α)-Stable.

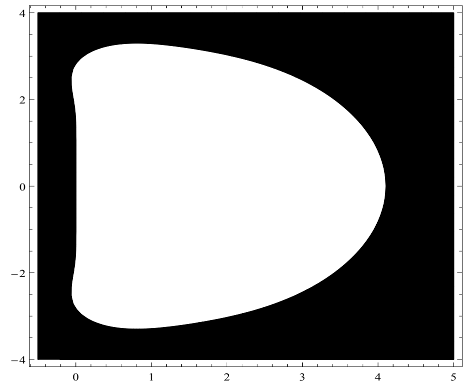

Figure 1: *RAS of SDBDF for* $k = 2$

4 Experimental Problems

Problem 5.2: A linear stiff problem

The linear system of 3 first order ordinary differential equations solved by Akinfenwa [1], Brugnano and Trigiante [3] and Ramos and Garcia-Rubio [22] given by,

$$\begin{array}{ll} {y_1}' = -21y_1 + 19y_2 - 20y_3, & y_1(0) = 1, \\ {y_2}' = 19y_1 - 21y_2 + 20y_3, & y_2(0) = 0, \\ {y_3}' = 40y_1 - 40y_2 + 40y_3, & y_2(0) = -1, \end{array} \quad (15)$$

on the interval $0 < x < 10$ is solved with the newly derived block multistep method. We compare the maximum absolute errors ($|y(x) - y_n|$) on the interval $0 < x < 10$ with the Adams Type Block method of Akinfenwa [1] of order $p = 7$ (ATBM7) and Generalized Backward Differentiation formula of Brugnano and Trigiante [3] (GBDF8) using step lengths $h = \frac{1}{2^n \cdot 100}$, $n = 0, 1, 2, 3$ and 4 for numerical solution of $y(x)$. The order of the methods are also verified by calculating the rate of convergence with the formula

$$Rate_h = log_2 \left(\frac{err_{2h}}{err_h} \right),$$

where err_h is the maximum absolute error at step length h.

Also in the range $0 \leq x \leq 1$, AbsErr(t_f) in [22] is obtained by the new method in comparison with the $CBDF_5$ of degree $s = 5$ in Ramos and Garcia-Rubio [22] and the following results are presented

Remark 4.1: Clearly from Table 2, it can be seen that the new method even though it is of order $p = 5$, performs better that the ATBM7 and the GBDF8, both of orders 7 and 8 respectively. Also, the rate of convergence of the new method conforms almost exactly with the order of our methods unlike the ATBM7 and GBDF8. Table 2 shows that the new method is comparable with the $CBDF_5$ in [22]. Numerical results also show that the new method is consistent with order of the method as the step size decreases.

Table 1: Problem 4.1: Maximum Absolute Error: $\max_{1<i<N} |y_1(x) - y_1, n|$ for $h = \frac{1}{2^n \cdot 100}$

n	New Method (Rate)	GBDF8 (Rate)	ATBM7 (Rate)
0	3.21×10^{-13}	1.19×10^{-3}	3.95×10^{-6}
1	1.01×10^{-14} (4.99)	1.39×10^{-5} (6.42)	2.91×10^{-8} (7.08)
2	3.18×10^{-16} (4.99)	1.08×10^{-7} (7.00)	2.21×10^{-10} (7.06)
3	9.96×10^{-18} (5.00)	1.08×10^{-9} (6.64)	6.65×10^{-13} (8.36)
4	3.11×10^{-19} (5.00)	9.41×10^{12} (6.84)	2.69×10^{-15} (7.95)

Table 2: Problem 4.1: Numerical Results in comparison with $CBDF_5$ in the range $0 \leq x \leq 1$

Steps	New Method	Rate	$CBDF_5$	Rate
20	3.04×10^{-11}		4.12×10^{-12}	
40	9.75×10^{-13}	4.96	1.33×10^{-12}	4.95
80	2.25×10^{-14}	5.43	4.31×10^{-15}	4.95
160	9.69×10^{-16}	4.53	2.55×10^{-15}	0.75

Problem 4.2: Cash [4].

We also consider the integration of the stiff system using the problem whose Jacobian matrix J has imaginary eigenvalues given by

$$\begin{array}{ll} {y_1}' = -\alpha y_1 - \beta y_2 + (\alpha + \beta - 1)e^{-t}, & y_1(0) = 1, \\ {y_2}' = \beta y_1 - \alpha y_2 + (\alpha - \beta - 1)e^{-t}, & y_2(0) = 1, \\ & 0 \leq t \leq 20, \end{array} \quad (16)$$

It is noted that for any given value of parameter α and β, J is the matrix,

$$\begin{pmatrix} -\alpha & -\beta \\ \beta & -\alpha \end{pmatrix},$$

with eigenvalues of J as $-\alpha \pm i\beta$ and the required solution is

$$\begin{aligned} y_1(t) &= e^{-t}, \\ y_2(t) &= e^{-t}, \end{aligned}$$

For the case $\alpha = 1$ and $\beta = 15$ with a fixed step size

$h = 0.25$, Table 3 presents the results obtained by the new method in comparison with the results in Cash [4] for the second derivative extended backward differentiation formulas (E2BD).

Table 3: Numerical Results for Problem 4.2, $x.xx(-xx) = x.xx \times 10^{-xx}$

t	E2BD		SDBDFC2New Method	
	$\|y_1 - y_1(t)\|$	$\|y_2 - y_2(t)\|$	$\|y_1 - y_1(t)\|$	$\|y_2 - y_2(t)\|$
5.0	0.879(-9)	0.353(-8)	0.147(-8)	0.363(-9)
10.0	0.459(-11)	0.237(-10)	0.994(-11)	0.245(-11)
15.0	0.401(-13)	0.160(-12)	0.670(-13)	0.165(-13)
20.0	0.270(-15)	0.108(-14)	0.451(-15)	0.111(-15)

Remark 4.2: Table 3 shows clearly that the new method on implementation on Problem 4.2 compares favourably with the method E2BD as obtained in Cash [4].

Problem 4.3: Stability test of Chartier [6]

The stability of the method is compared with L-Stable method of order 5 of Chartier [6] and the Backward Differentiation Formula of order 5 (BDF5) using the problem whose Jacobian matrix J has purely imaginary eigenvalues:

$$\begin{array}{ll} {y_1}' = -\alpha y_2 + (1+\alpha)\cos x, & y_1(0) = 0, \\ {y_2}' = \alpha y_1 - (1+\alpha)\sin x, & y_2(0) = 1, \\ & 0 \le x \le 100, \end{array} \tag{17}$$

with exact solution,

$$\begin{array}{rcl} y_1(x) & = & \sin x, \\ y_2(x) & = & \cos x. \end{array}$$

It is noted that for any given value of parameter α, J is the matrix,

$$\begin{pmatrix} 0 & -\alpha \\ \alpha & 0 \end{pmatrix},$$

with eigenvalues of J are $i \cdot \alpha$ and $-i \cdot \alpha$. For $\alpha = 10$, we present in Table 4 the accurate digits Δ , which is defined as,

$$\Delta = -\log_{10} \frac{\|y_i(x) - y_{n,i}\|_\infty}{\|y_{n,i}\|_\infty}$$

for the following methods defined by acronyms:

- $M(5, r_5)$- Chartier [6] order at least $p = 5$
- BDF5-Gear [14] Backward Differentiation Formula of order $p = 5$

Remark 4.3: Numerical overflow is indicated by ∞. Table 4 shows that the new method gained some digits and behaves correctly over other methods.

Table 4: Problem 4.3: Table of Accurate Digits Δ with $\alpha = 10$ for methods of Order $p = 5$

h	New Method	$M(5, r_5)$	BDF5
$\frac{4}{5}$	4.53	2.58	-0.41
$\frac{2}{5}$	5.63	3.66	∞
$\frac{1}{10}$	8.83	5.98	∞
$\frac{1}{20}$	10.46	7.22	8.15
$\frac{1}{40}$	12.00	8.14	10.00

5 Conclusion

In this paper, the construction of L(α)-stable block multistep method for solving stiff initial value problem is described. We have Investigated some numerical properties of the method that the methods are uniformly accurate of order $p = 5$ and further analysis reveals that the method possesses some stiff stability properties with good region of absolute stability. Implementation on some stiff problems shows that a class of order $p = 5$ performs better than methods of order $p = 8$ in the literature, and could be competitive with some stiff codes for solving stiff problems.

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