

SECOND DERIVATIVE PARALLEL MULTI-BLOCK METHODS FOR STIFF ODEs

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Abstract

A general theoretical background for second derivative multi-block methods and off-node form of block method developed in a previous study are presented herein. The proposed off-node block methods are L-stable for $k \leq 7$. Numerical results are included to justify their application on stiff IVPs in ODEs.

Keywords: Block methods, Off-node methods, Stiff IVPs.

1. INTRODUCTION

Numerical methods for integrating stiff initial value problems (IVPs) in ordinary differential equations (ODEs) of the form

$$y' = f(y(x)) \quad , f : \mathbb{R}^n \rightarrow \mathbb{R}^n, y(x_0) = y_0 \quad (1)$$

on parallel computers are currently receiving huge research interest. Among these methods are the parallel block methods developed in [1-7]. Chu and Hamilton [1] defined r-block k-point block methods as:

$$Y_m = \sum_{i=1}^r A_i Y_{m-i} + h \sum_{i=0}^r B_i F_{m-i} \quad (2)$$

where $A_i, B_i, i = 0, 1, \dots, r$ are $k \times k$ matrices, Y_m, F_m are vectors of the solution and its derivatives respectively (see [1]). If $k = 1$, then (2) is the classical linear multi-step method (LMM) of r -step method.

Sommeijer et al [6] developed methods of the form (2) for $r=1$, such methods are called One-block k -point methods. Classical r -step methods for integrating stiff IVP (1) are necessarily implicit. However, Dahlquist order barrier places severe restriction on the order an A-stable LMM can attain (see [8-11]). In [12], Dahlquist order barrier is circumvented by developing LMMs that incorporate the second derivative component ($y'' = \frac{d^2y}{dx^2}$) directly into their formulas.

Methods whose formulas contain second derivative components are called second derivative LMM ([2], [3], [9], [10], [11], [12]). In [12], the second derivative LMM is thus given as:

$$y_{n+1} = \sum_{i=1}^r a_i y_{n+1-i} + h \sum_{i=0}^r b_i f_{n+1-i} + h^2 \sum_{i=0}^r d_i f'_{n+1-i}. \quad (3)$$

In this paper a straight forward generalization of (3) to multi-block methods is given. This paper is organized as follows: section 2 is on the theory of second derivative multi-block methods for the IVP (1); Off-node second derivative parallel block backward differentiation type formulas are developed in Section 3. Section 4, is on the stability of off-node second derivative parallel block backward differentiation type formulas. Numerical experiment is performed in section 5, in section 6, is the conclusion.

2. Theory of Second Derivative Multi-Block Methods.

Let y_{n+i} denote the numerical approximate to the solution value $y(x_{n+i})$ of (1). By introducing the k -vectors

$$Y_{m-i} = \begin{pmatrix} y_{n-ik+c_1} \\ y_{n-ik+c_2} \\ \vdots \\ y_{n-k(i-c_k)} \end{pmatrix}, F(Y_{m-i}) = \begin{pmatrix} f_{n-ik+c_1} \\ f_{n-ik+c_2} \\ \vdots \\ f_{n-k(i-c_k)} \end{pmatrix} \text{ and } F'(Y_{m-i}) = \begin{pmatrix} f'_{n-ik+c_1} \\ f'_{n-ik+c_2} \\ \vdots \\ f'_{n-k(i-c_k)} \end{pmatrix}, \quad (4a)$$

$i = 0, 1, 2, \dots, r$. The (3) can be generalized into the second derivative r-block k-point block. The block formalism of (3) is given by the finite difference equation

$$\sum_{i=0}^r A_i Y_{m-i} = h \sum_{i=0}^r B_i F_{m-i} + h^2 \sum_{i=0}^r D_i F'_{m-i} \quad (4b)$$

where A_i, B_i and D_i , $i = 0, 1, \dots, r$ are carefully chosen k-by-k matrices. A_0 is an k-by-k unit matrix and h the step-length. The second derivative r-block, k-point method (4b) is explicit; if the coefficient matrices B_0 and D_0 , are null or strictly lower triangular otherwise it is implicit.

DEFINITION 1

Method (4b) is said to be parallel if the matrices B_0 and D_0 are diagonal matrices.

DEFINITION 2

Let $Z_{m-i} = (y(x_{n-ik+1}) \ y(x_{n-ik+2}) \ \dots \ y(x_{n-k(i-1)}))^T$, $i = 0, 1, \dots, r$, be the theoretical solution to

(1). The local truncation error (l.t.e) of (4b) is given by the vector E_m :

$$E_m = Z_m - \sum_{i=1}^r A_i Y_{m-i} - h \sum_{i=0}^r B_i F_{m-i} - h^2 \sum_{i=0}^r D_i F'_{m-i} \quad (5)$$

DEFINITION 3

The second derivative block method (4b) has error order $p \geq 1$ provided there exist a constant C such that the local truncation error E_m satisfies:

$$\|E_m\| = Ch^{p+1} Y^{(p+1)}(x_n^*) + O(h^{p+2}), \quad x_n \leq x^* \leq x_{n+1} \quad (6)$$

where $\|\cdot\|$ may be the maximum norm, the C is called the error constant of (4b).

DEFINITION 4

The second derivative block method (4b) is zero stable if the roots $R_j, j = 1, 2, \dots, r$ of the first characteristics polynomial

$$\rho(R) = \det\left(\sum_{i=1}^r A_i R^{r-i}\right) = 0 \quad (7)$$

satisfies $|R_j| \leq 1$, with $|R_j| = 1$ is simple.

When (4b) is applied to the test equation

$$y' = \lambda y, \text{ with } \operatorname{Re}(\lambda) < 0 \quad (8)$$

yields the characteristic equation

$$\pi(R, \mu) = \det\left(\sum_{i=0}^r A_i R^{r-i} - \mu \sum_{i=0}^r B_i R^{r-i} - \mu^2 \sum_{i=0}^r D_i R^{r-i}\right) = 0 \quad (9a)$$

where $\mu = \lambda h$. By Setting $\rho(R) = \sum_{i=0}^r A_i R^{r-i}$, $\sigma(R) = \sum_{i=0}^r B_i R^{r-i}$ and $\gamma(R) = \sum_{i=0}^r D_i R^{r-i}$,

we rewrite (9a) as

$$\pi(R, \mu) = \det(\rho(R) - \mu\sigma(R) - \mu^2\gamma(R)) = 0 \quad (9b)$$

The stability region associated with (4b) is the set

$$Z = \{\mu : \text{all roots } R_j(\mu); j = 1(1)r \text{ of (9b) are such that } |R_j(\mu)| \leq 1\}$$

DEFINITION 5

The second derivative block method (4b) is A-stable if the stability region Z contains the entire left half plane $\mathbf{C}^- = \{\mu \in \mathbf{C}; \operatorname{Re}(\mu) < 0\}$.

DEFINITION 6

The second derivative block method (4b) is L-stable, if it is A-stable and in addition (9b) has vanishing roots as $\mu \rightarrow -\infty$.

3. Off-node Block Method.

In [2], second derivative parallel block backward differentiation type formulas (SDBBDF) which is given as:

$$Y_m = A_1 Y_{m-1} + h B_0 F(Y_m) + h^2 D_0 F'(Y_m), \quad (10)$$

where B_0 , and D_0 are diagonal matrices and k -vectors as specified in (4a). The SDBBDF (10) is a generalization of one-step second derivative backward differentiation formulas (SDBDF) developed in [10]. In this paper, we present off-node SDBBDF a variant of SDBBDF (10). The c_i 's in (4a) for SDBBDF (10) are given as $c_i = i, i = 1(1)k$; by specifying the k -vectors as

$$Y_{m-1} = \begin{pmatrix} y_{n-(k-1)} \\ y_{n-(k-2)} \\ \vdots \\ y_n \end{pmatrix}, Y_m = \begin{pmatrix} y_{n+c_1} \\ y_{n+c_2} \\ \vdots \\ y_{n+c_k} \end{pmatrix}, F(Y_m) = \begin{pmatrix} f_{n+c_1} \\ f_{n+c_2} \\ \vdots \\ f_{n+c_k} \end{pmatrix} \text{ and } F'(Y_m) = \begin{pmatrix} f'_{n+c_1} \\ f'_{n+c_2} \\ \vdots \\ f'_{n+c_k} \end{pmatrix}, c_i = \frac{i}{k}, i = 1(1)k; \quad (11)$$

an off-node variant of SDBBDF (10) is developed. Substituting (11) into (10) and using methods of undetermined coefficients and Taylor's series expansion, elements of A_1, B_0 , and D_0 are determined. In what follows, we present coefficient matrices A_1, B_0 , and D_0 for proposed off-node SDBBDF for block sizes $k \leq 7$.

Two Point Block Method

$$A_1 = \begin{pmatrix} -\frac{1}{26} & \frac{27}{26} \\ -\frac{1}{7} & \frac{8}{7} \end{pmatrix}, B_0 = \begin{pmatrix} \frac{6}{13} & 0 \\ 0 & \frac{6}{7} \end{pmatrix}, D_0 = \begin{pmatrix} -\frac{9}{104} & 0 \\ 0 & -\frac{2}{7} \end{pmatrix}, C_4 = \begin{pmatrix} \frac{9}{1664} & \frac{1}{21} \end{pmatrix}^T, p = 3. \quad (12)$$

Three Point Block Method

$$A_1 = \begin{pmatrix} \frac{32}{10665} & -\frac{343}{10665} & \frac{10976}{10665} \\ \frac{125}{7101} & -\frac{1024}{7101} & \frac{8000}{7101} \\ \frac{4}{85} & -\frac{27}{85} & \frac{108}{85} \end{pmatrix}, B_0 = \begin{pmatrix} \frac{364}{1185} & 0 & 0 \\ 0 & \frac{440}{789} & 0 \\ 0 & 0 & \frac{66}{85} \end{pmatrix}, D_0 = \begin{pmatrix} -\frac{392}{10665} & 0 & 0 \\ 0 & -\frac{800}{7101} & 0 \\ 0 & 0 & -\frac{18}{85} \end{pmatrix},$$

$$C_5 = \left(\frac{2267}{4483350} \quad \frac{36346}{9436905} \quad \frac{9}{425} \right)^T, p = 4 \quad (13)$$

Four Point Block Method

$$A_1 = \begin{pmatrix} -\frac{30375}{65376512} & \frac{274625}{65376512} & -\frac{1601613}{65376512} & \frac{66733875}{65376512} \\ \frac{1125}{351136} & \frac{9261}{351136} & -\frac{42875}{351136} & \frac{385875}{351136} \\ -\frac{456533}{46606592} & \frac{3472875}{46606592} & -\frac{13476375}{46606592} & \frac{57066625}{46606592} \\ \frac{9}{415} & \frac{64}{415} & -\frac{216}{415} & \frac{576}{415} \end{pmatrix}, B_0 = \begin{pmatrix} \frac{118755}{510754} & 0 & 0 & 0 \\ 0 & \frac{4620}{10973} & 0 & 0 \\ 0 & 0 & \frac{211365}{364114} & 0 \\ 0 & 0 & 0 & \frac{60}{83} \end{pmatrix},$$

$$D_0 = \begin{pmatrix} -\frac{342225}{16344128} & 0 & 0 & 0 \\ 0 & -\frac{11025}{175568} & 0 & 0 \\ 0 & 0 & -\frac{1334025}{11651648} & 0 \\ 0 & 0 & 0 & -\frac{72}{415} \end{pmatrix}$$

$$C_6 = \left(\frac{4448925}{33472774144} \quad \frac{25725}{22472704} \quad \frac{102719925}{23862575104} \quad \frac{24}{2075} \right)^T, p = 5. \quad (14)$$

Five Point Block Method

$$A_1 = \begin{pmatrix} \frac{144}{12019} & -\frac{1125}{12019} & \frac{4000}{12019} & -\frac{9000}{12019} & \frac{18000}{12019} \\ \frac{60665724}{74990603125} & \frac{525926016}{74990603125} & \frac{2242946629}{74990603125} & \frac{7533161856}{74990603125} & \frac{8074607644}{74990603125} \\ \frac{205006464}{78201353125} & \frac{1710777536}{78201353125} & \frac{6811962624}{78201353125} & \frac{19486825371}{78201353125} & \frac{92381986944}{78201353125} \\ \frac{63521199}{10373884375} & \frac{512096256}{10373884375} & \frac{1920081024}{10373884375} & \frac{4818200576}{10373884375} & \frac{13720578984}{10373884375} \\ \frac{144}{12019} & -\frac{1125}{12019} & \frac{4000}{12019} & -\frac{9000}{12019} & \frac{18000}{12019} \end{pmatrix}$$

$$B_0 = \begin{pmatrix} \frac{3736656}{19895065} & 0 & 0 & 0 & 0 \\ 0 & \frac{40982172}{119984965} & 0 & 0 & 0 \\ 0 & 0 & \frac{58792968}{125122165} & 0 & 0 \\ 0 & 0 & 0 & \frac{9662184}{16598215} & 0 \\ 0 & 0 & 0 & 0 & \frac{8220}{12019} \end{pmatrix}$$

$$D_0 = \begin{pmatrix} -\frac{6830208}{497376625} & 0 & 0 & 0 & 0 \\ 0 & -\frac{123370632}{2999624125} & 0 & 0 & 0 \\ 0 & 0 & -\frac{231727392}{3128054125} & 0 & 0 \\ 0 & 0 & 0 & -\frac{45849888}{414955375} & 0 \\ 0 & 0 & 0 & 0 & -\frac{1800}{12019} \end{pmatrix}$$

$$C_7 = \left(\frac{300529152}{7771509765625}, \frac{15380205456}{46869126953125}, \frac{415718941248}{341230919921875}, \frac{20907548928}{6483677734375}, \frac{600}{84133} \right)^T, p = 6 \quad (15)$$

Six Point Block Method

$$A_1 = \begin{pmatrix} \frac{16152323403125}{475805888841671424} & \frac{153982037280799}{475805888841671424} & \frac{350775525953125}{237902944420835712} & \frac{1095115763546875}{237902944420835712} & \frac{7014487849890625}{475805888841671424} & \frac{481193866502496875}{475805888841671424} \\ \frac{18839275}{72771950421} & \frac{175616000}{72771950421} & \frac{771656704}{72771950421} & \frac{2249728000}{72771950421} & \frac{6028568000}{72771950421} & \frac{77165670400}{72771950421} \\ \frac{6251175}{7253380864} & \frac{57066625}{7253380864} & \frac{121287375}{3626690432} & \frac{332812557}{3626690432} & \frac{1540798875}{7253380864} & \frac{8320313925}{7253380864} \\ \frac{2921811200}{1415916119601} & \frac{26156812000}{1415916119601} & \frac{107850176000}{1415916119601} & \frac{280368328625}{1415916119601} & \frac{574194337024}{1415916119601} & \frac{1794357303200}{1415916119601} \\ \frac{1940449395472489}{469116106139167488} & \frac{17056207271901875}{469116106139167488} & \frac{34189515834175625}{234558053069583744} & \frac{84670026288299375}{234558053069583744} & \frac{312534815292573125}{469116106139167488} & \frac{665574142647063727}{469116106139167488} \\ \frac{100}{13489} & \frac{864}{13489} & \frac{3375}{13489} & \frac{8000}{13489} & \frac{13500}{13489} & \frac{21600}{13489} \end{pmatrix}$$

$$B_0 = \begin{pmatrix} \frac{402399852400}{2549542871451} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{28836080}{99824349} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{11275110}{28333519} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{956041240}{1942271769} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1449228745580}{2513696556387} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1260}{1927} \end{pmatrix}$$

$$D_0 = \begin{pmatrix} \frac{1795533000625}{183567086744472} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{26499200}{898419141} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{12006225}{226668152} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1370784800}{17480445921} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{19057721215225}{180986152059864} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{1800}{13489} \end{pmatrix}$$

$$C_8 = \left(\frac{68741980928928125}{4933155455510449324032} \quad \frac{688979200}{5894527984101} \quad \frac{396205425}{928432750592} \quad \frac{128168378800}{114689205687681} \quad \frac{11885252547268995125}{4863795788450888515584} \quad \frac{450}{94423} \right)^T, P=7$$

(16)

Seven Point Block Method

$$A_1 = \left(\begin{array}{cccc}
\begin{array}{r}
50484527596800 \\
\hline
3979138943535030331 \\
239615515828800 \\
\hline
2433789106808380069 \\
128499849241216 \\
\hline
386983472658061993 \\
9095453452800000 \\
\hline
11310800211882887401 \\
5776455114144000 \\
\hline
3544427205628291423 \\
13558009322803725 \\
\hline
4589917074183198541 \\
3600 \\
\hline
726301
\end{array}
&
\begin{array}{r}
516187414562600 \\
\hline
3979138943535030331 \\
2417792600678400 \\
\hline
2433789106808380069 \\
1280385124884000 \\
\hline
386983472658061993 \\
89547874099200000 \\
\hline
11310800211882887401 \\
56224584310853673 \\
\hline
3544427205628291423 \\
130532699789107200 \\
\hline
4589917074183198541 \\
34300 \\
\hline
726301
\end{array}
&
\begin{array}{r}
2468658002976000 \\
\hline
3979138943535030331 \\
11339671166866944 \\
\hline
2433789106808380069 \\
5895848794320000 \\
\hline
386983472658061993 \\
405265071387515625 \\
\hline
11310800211882887401 \\
250325110324640000 \\
\hline
3544427205628291423 \\
572234645466432000 \\
\hline
4589917074183198541 \\
148176 \\
\hline
726301
\end{array}
&
\begin{array}{r}
7539206115024000 \\
\hline
3979138943535030331 \\
33552080381952000 \\
\hline
2433789106808380069 \\
16940898093324375 \\
\hline
386983472658061993 \\
1133203273320628224 \\
\hline
11310800211882887401 \\
68244071383224000 \\
\hline
3544427205628291423 \\
1523555725273088000 \\
\hline
4589917074183198541 \\
385875 \\
\hline
726301
\end{array} \\
\hline
\begin{array}{r}
17839437047283456 \\
\hline
3979138943535030331 \\
74748808961281125 \\
\hline
2433789106808380069 \\
35750708616240000 \\
\hline
386983472658061993 \\
2277044900416000000 \\
\hline
11310800211882887401 \\
1311551755319520000 \\
\hline
3544427205628291423 \\
2811388813176580416 \\
\hline
4589917074183198541 \\
686000 \\
\hline
726301
\end{array}
&
\begin{array}{r}
47037578152016925 \\
\hline
3979138943535030331 \\
167995128398028800 \\
\hline
2433789106808380069 \\
70257292572634848 \\
\hline
386983472658061993 \\
3990901835980800000 \\
\hline
11310800211882887401 \\
2082392011513099000 \\
\hline
3544427205628291423 \\
4094876741995929600 \\
\hline
4589917074183198541 \\
926100 \\
\hline
726301
\end{array}
&
\begin{array}{r}
4013873335638777600 \\
\hline
3979138943535030331 \\
2551426012545062400 \\
\hline
2433789106808380069 \\
433686991189104000 \\
\hline
386983472658061993 \\
13833047770027200000 \\
\hline
11310800211882887401 \\
4797831194526180096 \\
\hline
3544427205628291423 \\
6941700773275507200 \\
\hline
4589917074183198541 \\
1234800 \\
\hline
726301
\end{array}
\end{array} \right)$$

$$C_9 = \left(\frac{55748240772760800}{9553912603427607824731}, \frac{283491779171673600}{5843527645446920545669}, \frac{162632621695914000}{929147317852006845193}, \frac{12296042462246400000}{27157231308730812649801}, \right. \\ \left. \frac{8329568046052396000}{8510169720713527706623}, \frac{20825102319826521600}{11020390895113859696941}, \frac{2450}{726301} \right)^T \quad p = 8.$$

(17)

4. Stability Analysis of Proposed Off-node Block Methods.

The roots R of characteristic polynomial equation $\rho(R) = \det(I - A_1 R) = 0$, are eigenvalues of matrix A_1 . Eigenvalues of A_1 for methods with coefficient matrices in (12)-(17) are $R \leq 1$ and eigenvalues with $R=1$ being simple. Thus proposed off-node SDBBDF with coefficient matrices in (12)-(17) are zero stable. An A-stable block method of the form (10) is L-stable, see [2]. Therefore, A-stable off-node SDBBDF implies L-stable method. Applying our proposed off-node SDBBDF block methods (12)-(17) to the test equation (8) yield the characteristic polynomial defined by

$$\pi(R, \mu) = \det(IR - A_1 - \mu B_0 R - \mu^2 D_0 R) = 0. \quad (18)$$

The boundary locus of the characteristics roots for block sizes $k \leq 7$ are shown in figures (1)-(6)

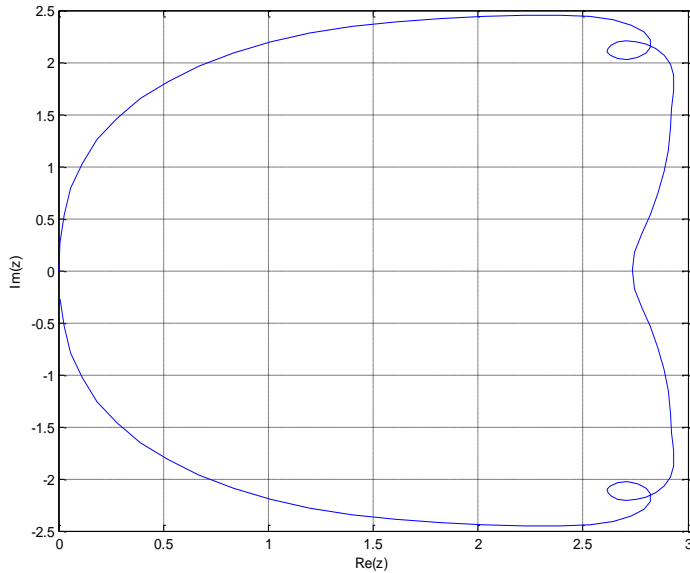


Fig. (1): Stability Region of Off-node SDBBDF (12)

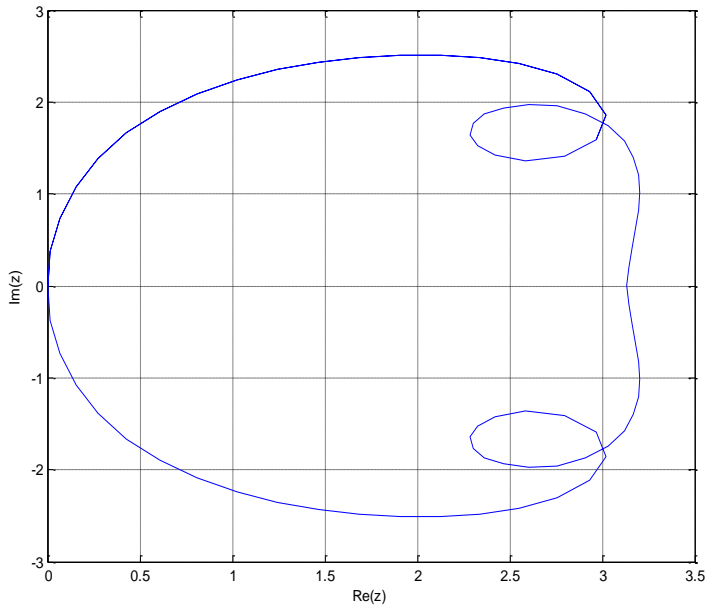


Fig. (2): Stability Region of Off-node SDBBDF (13)

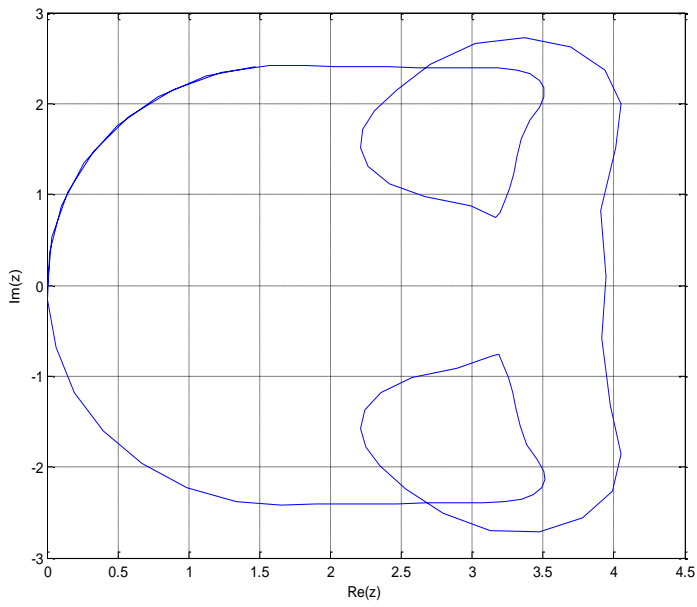


Fig. (3): Stability Region of Off-node SDBBDF (14)

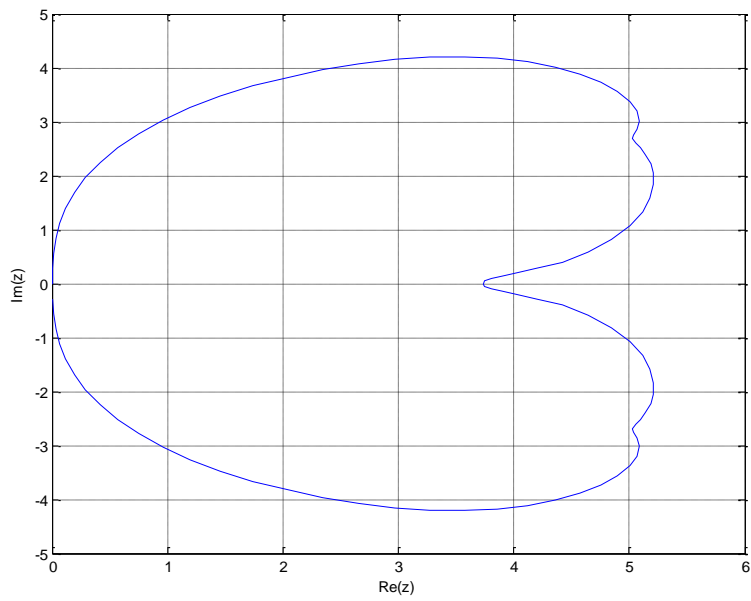


Fig. (4): Stability Region of Off-node SDBBDF (15)

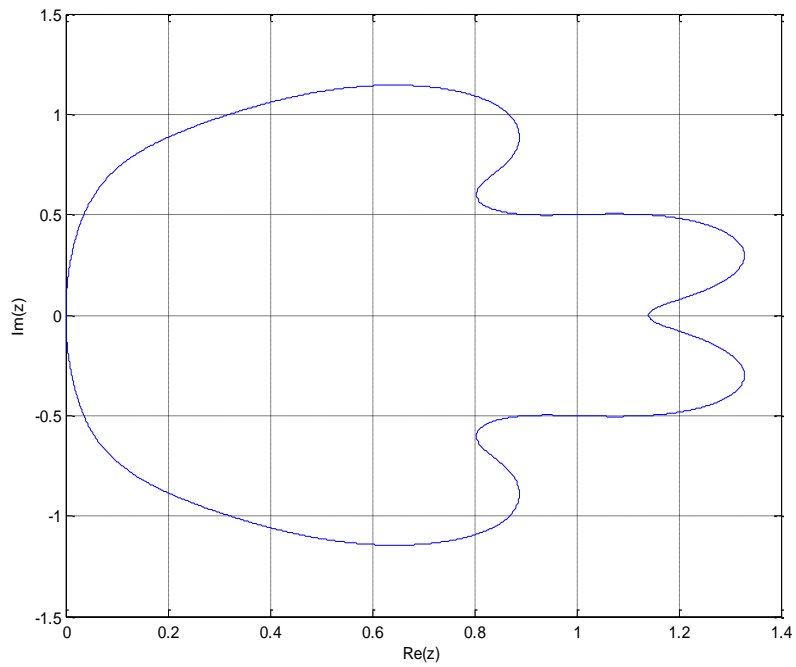


Fig. (5): Stability Region of Off-node SDBBDF (16)

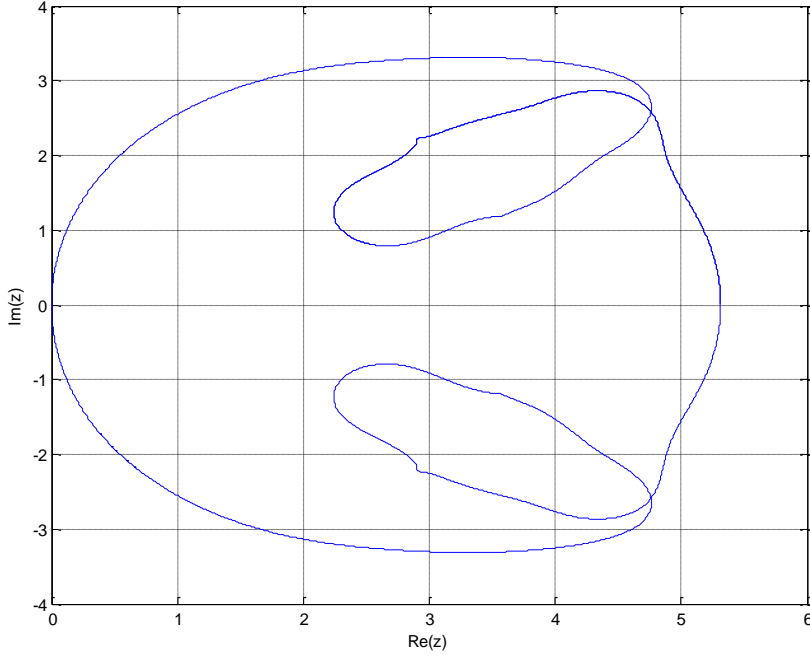


Fig. (6): Stability Region of Off-node SDBBDF (17)

Observe from figures (1)–(6), that the regions of absolute stability for block sizes $k \leq 7$ include the entire left of the complex plane, thus our proposed off-node SDBBDF are A-stable and hence L-stable for block sizes $k \leq 7$. In [4], construction and prove for L-stable off-node SDBBDF of block size $k=8$ is shown.

5. Numerical Experiments

In this section, we tested the proposed off-node block size $k=2$ on the stiff problem (see [13])

$$y' = \begin{pmatrix} -10 & \alpha & 0 & 0 & 0 & 0 \\ -\alpha & -10 & 0 & 0 & 0 & 0 \\ 0 & 0 & -4 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & -0.1 \end{pmatrix} y, \quad y(x) = \begin{pmatrix} e^{-10x} (\cos(\alpha x) + \sin(\alpha x)) \\ e^{-10x} (\cos(\alpha x) - \sin(\alpha x)) \\ e^{-4x} \\ e^{-x} \\ e^{-0.5x} \\ e^{-0.1x} \end{pmatrix}, \quad y(0) = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad 0 \leq x \leq 3.$$

Using a fixed step-size $h=0.01$ and inverse Euler's method in [9] to generate starting values. The plots of numerical solution generated by proposed off-node SDBBDF compared with numerical

solutions generated by SDBBDF of block size $k=2$ and SDBDF of step-size $k=2$ are shown in figure 7.

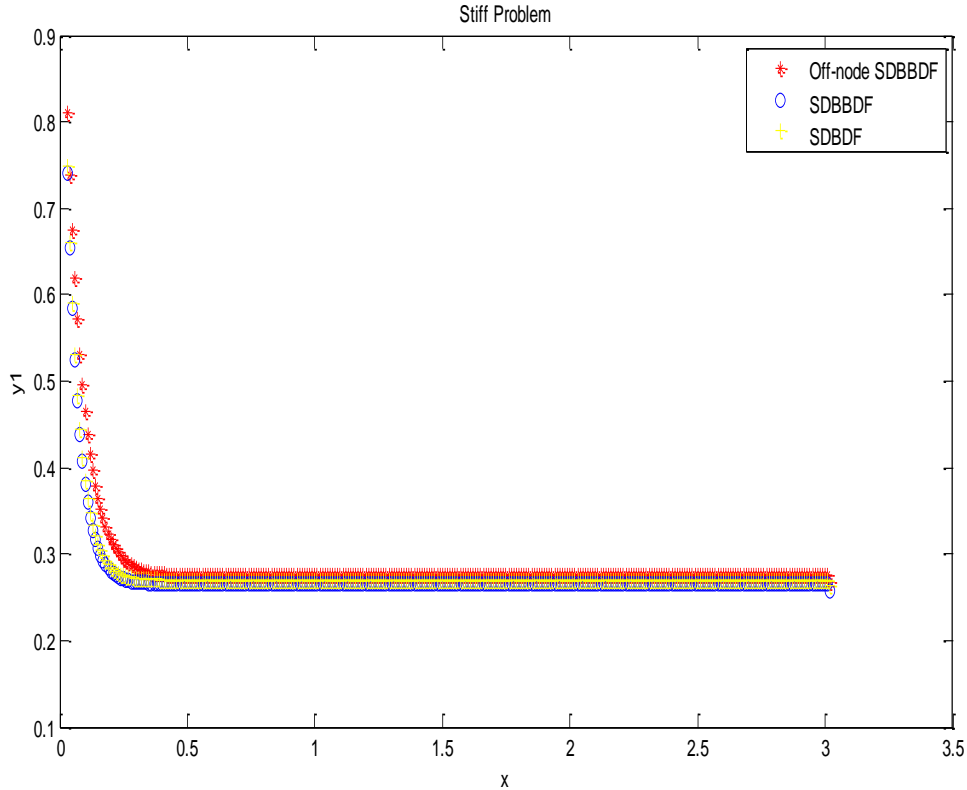


Fig. (7): y_1 Component Generated by Off-node SDBBDF, SDBBDF and SDBDF

From figure (7), the numerical solution of stiff problem generated by proposed off-node SDBBDF compares favourable with SDBBDF and SDBDF.

6. Conclusion

Theory on second derivative multi-block methods is developed, in addition off-node SDBBDF a variant of SDBBDF developed in [2] is proposed. The family of off-node SDBBDF has higher order L-stable methods compared to family of SDBBDF. The numerical result shows that the proposed off-node SDBBDF is suitable for integrating stiff IVPs in ODEs (1).

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