Acta Univ. Palacki. Olomuc., Fac. rer. nat.,
Mathematica **51**, 1 (2012) 51–77

The Numerical Solution of Stiff IVPs in ODEs Using Modified Second Derivative BDF

R. I. OKUONGHAE[1], M. N. O. IKHILE[2]

Department of Mathematics, University of Benin
Benin City, P.M.B 1154, Edo state, Nigeria
[1]*e-mail: okunoghae01@yahoo.co.uk*
[2]*e-mail: mnoikhilo@yahoo.com*

(Received March 23, 2011)

Abstract

This paper considers modified second derivative BDF (MSD-BDF) for the numerical solution of stiff initial value problems (IVPs) in ordinary differential equations (ODEs). The methods are A(α)-stable for step length $k \leq 7$.

Key words: second derivative BDF, collocation and interpolation, initial value problem, stiff stability, boundary locus

2000 Mathematics Subject Classification: 65L05, 65L06

1 Introduction

In [30], a class of $A(\alpha)$ stable linear multistep method

$$y(x_n + (t+1)h) = \sum_{j=0}^{k-1} \alpha_{k,j}(t) y_{n+j} + h\beta_{k,v}(t) f_{n+v} + h^2 \gamma_{k,v}(t) f'_{n+v}, \quad t = k-1, \quad v = k - \frac{1}{2}, \tag{1}$$

with hybrid predictor

$$y(x_n + vh) = \sum_{j=0}^{k-1} \alpha_{2,j}(t) y_{n+j} + h\phi_k(t) f_{n+k} + h^2 \delta_k(t) f'_{n+k}, \quad v = t+1,\ t = k - \frac{3}{2}, \tag{2}$$

was considered for the numerical solution of stiff initial value problems (IVPs) in ordinary differential equations (ODEs)

$$\begin{aligned} y' &= f(x, y), \ x \in [x_0, X], \\ y(x_0) &= y_0. \end{aligned} \tag{3}$$

$f: \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$. The scheme in (1) with hybrid predictor (2) were found to be $A(\alpha)$ stable for $k \leq 6$ and unstable for $k \geq 7$. In this paper, we consider another scheme called the Modified Second Derivative Backward Differentiation Formula (MSD-BDF). The new method produces approximate solution y_n to $y(x_n)$ at the end of a step $[x_{n+t}, x_{n+t+1}]$ of length $h = x_{n+1} - x_n$ according to

$$y(x_n + (t+1)h) = \sum_{j=0}^{k-1} \alpha_{k,j}(t) y_{n+j} + h\beta_{k,v}(t) f_{n+v} + h^2 \gamma_{k,v}(t) f'_{n+v} \tag{4}$$

with the hybrid predictor given as

$$y(x_n + vh) = \sum_{j=0}^{k} \alpha_j(t) y_{n+j} + h\phi_k(t) f_{n+k}. \tag{5}$$

The t and v in (4) and (5) are respectively fixed as

$$t = k - 1, \quad v = k - \frac{1}{2}, \tag{6}$$

and

$$v = t + 1, \quad t = k - \frac{3}{2}, \tag{7}$$

for each $n = 0, 1, 2, \ldots$ and $f_{n+j} = f(x_{n+j}, y_{n+j})$, $x = x_{n+1} + th$. Also, $\{\alpha_{k,j}(t), j = 0(1)k-1\}$, $\gamma_{k,v}(t)$, $\{\alpha_{2,j}(t), j = 0(1)k\}$, $\beta_{k,v}(t)$, and $\phi_k(t)$ are the continuous coefficients in t presumed to be real and satisfying the normalization condition $\alpha_{k,k}(t) = 1$, and $\alpha_v(t) = 1$. Our interest in this paper is to derive schemes whose step number k and order p are higher than the methods obtained from (1) and (2) and still retain $A(\alpha)$-stability property. To achieve these aims we have modified the structure of the hybrid predictor in (2) by deleting $h^2\delta_k(t) f'_{n+k}$ from it. The methods in (4) and (5) are for continuous output of the solution of stiff IVPs (3). Stiff IVPs arise in large variety of applications areas notably, pharmaco kinetic theory, heat and mass transfer, biological sciences, especially in modeling of spread and control of diseases and etc. It is important to say at this point that the schemes are formulated on the basis that the IVPs satisfies the existence and uniqueness theorem, so that polynomial interpolation can be applied in the method's formulation. In recent time, some stiffly stable methods had been proposed, examples of such are in [4, 10, 5, 6], [13], [16], and [18, 19]. In [1], [16], [25], and [20], the ideas of Taylor's series method was used to derived LMM and it hybrid counterpart, other techniques for deriving LMM and its hybrid formulas for the numerical solution of (3) include the numerical differentiation method discussed in [18, 19], numerical integration technique used by [13], trees approach in [1, 2, 9, 6, 8] and collocation and interpolation method due to [11], [14], [26], [27], [28]-[30] and [31] respectively. In this paper, collocation and interpolation technique is used to derive the continuous version in (4) and (5) from which the proposed discrete version is obtained. Sections 2 and 3 give details of the derivation of the schemes. In section 4, we investigate the stability of the scheme in (4), and give examples of methods that are A-stable and stiffly stable for a fixed step number k. Finally in section 5 we discuss the implementation of these methods.

The local truncation errors for (4) and (5) are

$$\begin{aligned} L.T.E = \Big[& y(x_n + (t+1)h) - \sum_{j=0}^{k-1} \alpha_{k,j}(t) y(x_n + jh) \\ & - h\beta_{k,v}(t) y'(x_n + vh) - h^2 \gamma_{k,v}(t) y''(x_n + vh) \Big] \end{aligned} \tag{8}$$

and

$$L.T.E = \Big[y(x_n + vh) - \sum_{j=0}^{k} \alpha_j(t) y(x_n + jh) - h\phi_k(t) y'(x_n + kh) \Big] \tag{9}$$

The order of (4) and (5) are $k+1$ respectively. It is the purpose of this paper to construct continuous methods which aim at large intervals of absolute stability, zero-stability, high order and small error constant which by-passes the Dahlquist order barrier theorem in [12] for conventional LMM.

2 Derivation of the MSD-BDF method

Let the solution of the IVPs in (3) is be approximated by the polynomial

$$y(x) = \sum_{j=0}^{k+1} a_j x^j \tag{10}$$

where $\{a_j\}_{j=0}^{k+1}$ are the real parameter constants to be determined. From (10) we have

$$\begin{aligned} y'(x) &= f(x,y) = \sum_{j=1}^{k+1} j a_j x^{j-1}, \\ y''(x) &= f'(x,y) = \sum_{j=2}^{k+1} j(j-1) a_j x^{j-2}, \end{aligned} \tag{11}$$

Collocating (10) at $x = x_{n+v}$ and interpolating (11) at $x = x_{n+j}$, $j = 0(1)k-1$ and $x = x_{n+v}$, we obtain the linear system of equations

$$\begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & \cdots & x_n^{k+1} \\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 & \cdots & x_{n+1}^{k+1} \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot \\ 1 & x_{n+k-1} & x_{n+k-1}^2 & x_{n+k-1}^3 & \cdots & x_{n+k-1}^{k+1} \\ 0 & 1 & 2x_{n+v} & 3x_{n+v}^2 & \cdots & (k+1)x_{n+v}^k \\ 0 & 0 & 2 & 6x_{n+v} & \cdots & (k+1)(k)x_{n+v}^{k-1} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \cdot \\ \cdot \\ \cdot \\ a_{k-1} \\ a_k \\ a_{k+1} \end{pmatrix} = \begin{pmatrix} y_n \\ y_{n+1} \\ \cdot \\ \cdot \\ \cdot \\ y_{n+k-1} \\ f_{n+v} \\ f'_{n+v} \end{pmatrix} \tag{12}$$

where $\{x_{n+j} = x_n + jh\}_{j=1}^{k-1}$, $x_{n+v} = x_n + vh$, and $v = k - \frac{1}{2}$. Setting $x_n = 0$ in (12) and solving equation (12) for $a_j's$ using Gaussian elimination method and substituting the resulting values into (10) with $x = x_{n+1} + th$, yield the continuous method for $k \le 7$. Setting $t = k-1$ and $v = k-\frac{1}{2}$ in (4) as defined in (6) yield the discrete methods for $k \le 7$. Below are the continuous and discrete coefficients for the scheme in (4) for $k \le 7$. The continuous coefficients for $k = 1$ of order 2 in (4) is nicely obtained as

$$\alpha_{1,0}(t) = 1, \quad \alpha_{1,1}(t) = 1, \quad \beta_{1,\frac{1}{2}}(t) = 1 + t, \quad \gamma_{1,\frac{1}{2}}(t) = \frac{t}{2} + \frac{t^2}{2} \tag{13}$$

setting $t = 0$ in (13), we have the discrete coefficients of (4) for $k = 1$ as

$$\alpha_{1,0}(0) = 1, \quad \alpha_{1,1}(0) = 1, \quad \beta_{1,\frac{1}{2}}(0) = 1, \quad \gamma_{1,\frac{1}{2}}(0) = 0. \tag{14}$$

Again, fixing $k = 2$ and $v = k - \frac{1}{2}$ in (4) yield a method of order 3 continuous coefficients

$$\alpha_{2,0}(t) = -\frac{3t}{13} + \frac{6t^2}{13} - \frac{4t^3}{13}, \quad \alpha_{2,1}(t) = 1 + \frac{3t}{13} - \frac{6t^2}{13} + \frac{4t^3}{13}, \tag{15}$$

$$\beta_{2,\frac{3}{2}}(t) = \frac{10t}{13} + \frac{6t^2}{13} - \frac{4t^3}{13}, \qquad \gamma_{2,\frac{3}{2}}(t) = -\frac{7t}{26} + \frac{t^2}{26} + \frac{4t^3}{13}, \tag{16}$$

substituting $t = 1$ into (15)–(16) give the discrete coefficients to be

$$\alpha_{2,0}(1) = -\frac{1}{13}, \quad \alpha_{2,1}(1) = \frac{14}{13} \quad \beta_{2,\frac{3}{2}}(1) = \frac{12}{13}, \quad \gamma_{2,\frac{3}{2}}(1) = \frac{1}{13}. \tag{17}$$

Similarly, setting $k = 3$ in (4), yield a scheme of order 4, with continuous coefficients:

$$\alpha_{3,0}(t) = -\frac{81t}{394} + \frac{171t^2}{394} - \frac{58t^3}{197} + \frac{13t^4}{197}, \tag{18}$$

$$\alpha_{3,1}(t = 1 - \frac{216t}{197} - \frac{135t^2}{197} + \frac{216t^3}{197} - \frac{62t^4}{197}, \tag{19}$$

$$\alpha_{3,2}(t) = \frac{513t}{394} + \frac{99t^2}{394} - \frac{158t^3}{197} + \frac{49t^4}{197}, \tag{20}$$

$$\beta_{3,\frac{5}{2}}(t) = -\frac{100t}{197} + \frac{36t^2}{197} + \frac{100t^3}{197} - \frac{36t^4}{197}, \tag{21}$$

$$\gamma_{3,\frac{5}{2}}(t) = \frac{42t}{197} - \frac{23t^2}{197} - \frac{42t^3}{197} + \frac{23t^4}{197}, \tag{22}$$

replacing t in (18)–(22) by 2, we obtain the discrete coefficients of the method (4) as

$$\begin{gathered}\alpha_{3,0}(2) = \tfrac{5}{197}, \quad \alpha_{3,1}(2) = -\tfrac{39}{197}, \quad \alpha_{3,2}(2) = \tfrac{231}{197}, \quad \alpha_{3,3}(2) = 1, \\ \beta_{3,\frac{5}{2}}(2) = \tfrac{168}{197}, \quad \gamma_{3,\frac{5}{2}}(2) = \tfrac{24}{197}.\end{gathered} \tag{23}$$

Letting $k = 4$ in (4) give the continuous coefficients of order 5 as

$$\alpha_{4,0}(t) = -\frac{5900t}{32919} + \frac{13135t^2}{32919} - \frac{6777t^3}{21946} + \frac{6649t^4}{65838} - \frac{394t^5}{32919}, \tag{24}$$

$$\alpha_{4,1}(t) = 1 - \frac{26875t}{21946} - \frac{11075t^2}{21946} + \frac{25415t^3}{21946} - \frac{10871t^4}{21946} + \frac{730t^5}{10973}, \tag{25}$$

$$\alpha_{4,2}(t) = \frac{26650t}{10973} - \frac{5860t^2}{10973} - \frac{38819t^3}{21946} + \frac{22693t^4}{21946} - \frac{1754t^5}{10973}, \tag{26}$$

$$\alpha_{4,3}(t) = -\frac{67475t}{65838} + \frac{42115t^2}{65838} + \frac{20181t^3}{21946} - \frac{42115t^4}{65838} + \frac{3466t^5}{32919}, \tag{27}$$

$$\alpha_{4,4}(t) = 1, \tag{28}$$

$$\beta_{4,\frac{7}{2}}(t) = \frac{4848t}{10973} - \frac{3800t^2}{10973} - \frac{4160t^3}{10973} + \frac{3800t^4}{10973} - \frac{688t^5}{10973}, \tag{29}$$

$$\gamma_{4,\frac{7}{2}}(t) = -\frac{1970t}{10973} + \frac{1689t^2}{10973} + \frac{1618t^3}{10973} - \frac{1689t^4}{10973} + \frac{352t^5}{10973}. \tag{30}$$

Inserting $t = 3$ into (24)–(30) yields the following discrete coefficients:

$$\begin{gathered}\alpha_{4,0}(3) = -\tfrac{137}{1093}, \quad \alpha_{4,1}(3) = \tfrac{1040}{10973}, \quad \alpha_{4,2}(3) = -\tfrac{4002}{10973}, \\ \alpha_{4,3}(3), = \tfrac{14072}{10973}, \quad \alpha_{4,4}(3) = 1, \quad \beta_{4,\frac{7}{2}}(3) = \tfrac{8640}{10973}, \quad \gamma_{4,\frac{7}{2}}(3) = \tfrac{1704}{10973}.\end{gathered} \tag{31}$$

In like manner, fixing $k = 5$ in (4) give the continuous coefficients of method of order 6 to be

$$\alpha_{5,0}(t) = -\frac{1215739t}{7819884} + \frac{17281817t^2}{46919304} - \frac{7493533t^3}{23459652} + \frac{2030017t^4}{15639768} - \frac{147269t^5}{5864913} + \frac{10973t^6}{5864913}, \tag{32}$$

$$\alpha_{5,1}(t) = 1 - \frac{1783943t}{1303314} - \frac{136857t^2}{434438} + \frac{1589315t^3}{1303314} - \frac{877079t^4}{1303314} + \frac{32438t^5}{217219} - \frac{7832t^6}{651657}, \tag{33}$$

$$\alpha_{5,2}(t) = \frac{1212897t}{434438} - \frac{892661t^2}{868876} - \frac{414719t^3}{217219} + \frac{1298019t^4}{868876} - \frac{83120t^5}{217219} + \frac{7270t^6}{217219}, \tag{34}$$

$$\alpha_{5,3}(t) = -\frac{8856211t}{3909942} + \frac{23002567t^2}{11729826} + \frac{19955933t^3}{11729826} - \frac{7456717t^4}{3909942} + \frac{3306350t^5}{5864913} - \frac{316208t^6}{5864913}, \tag{35}$$

$$\alpha_{5,4}(t) = \frac{2599891t}{2606628} - \frac{1715105t^2}{1737752} - \frac{1804039t^3}{2606628} + \frac{4985819t^4}{5213256} - \frac{66321t^5}{217219} + \frac{19937t^6}{651657}, \tag{36}$$

$$\alpha_{5,5}(t) = 1, \tag{37}$$

$$\beta_{5,\frac{9}{2}}(t) = -\frac{266848t}{651657} + \frac{849520t^2}{1954971} + \frac{515120t^3}{1954971} - \frac{273040t^4}{651657} + \frac{285424t^5}{1954971} - \frac{30400t^6}{1954971}, \tag{38}$$

$$\gamma_{5,\frac{9}{2}}(t) = \frac{34048t}{217219} - \frac{112144t^2}{651657} - \frac{62600t^3}{651657} + \frac{35880t^4}{217219} - \frac{39544t^5}{651657} + \frac{4504t^6}{651657}, \tag{39}$$

substituting $t = 4$ into (32)–(39) gives,

$$\begin{gathered} \alpha_{5,0}(4) = \tfrac{14491}{1954971}, \quad \alpha_{5,1}(4) = -\tfrac{13055}{217219}, \quad \alpha_{5,2}(4) = \tfrac{49390}{217219}, \\ \alpha_{5,3}(4), = -\tfrac{1130590}{1954971}, \quad \alpha_{5,4}(4) = \tfrac{304895}{217219}, \quad \alpha_{5,5}(4) = 1, \\ \beta_{5,\frac{9}{2}}(4) = \tfrac{472960}{651657}, \quad \gamma_{5,\frac{9}{2}}(4) = \tfrac{39680}{217219}. \end{gathered} \tag{40}$$

Setting $k = 6$, we have the continuous coefficients of the method (4) to be,

$$\alpha_{6,0}(t) = -\frac{19290069t}{141667595} + \frac{193448871t^2}{566670380} - \frac{368244713t^3}{1133340760} + \frac{26122729t^4}{170001114} - \frac{131446469t^5}{3400022280} + \frac{8431667t^6}{1700011140} - \frac{217219t^7}{850005570}, \tag{41}$$

$$\begin{aligned}
\alpha_{6,1}(t) &= 1-\frac{170790345t}{113334076}-\frac{27438479t^2}{226668152}+\frac{7696982581t^3}{6120040104}-\frac{1722620983t^4}{2040013368}\\
&\quad+\frac{1514216965t^5}{6120040104}-\frac{35223037t^6}{1020006684}+\frac{2869771t^7}{1530010026}, \qquad (42)\\
\alpha_{6,2}(t) &= \frac{91167282t}{28333519}-\frac{92394891t^2}{56667038}-\frac{229040863t^3}{113334076}+\frac{344335331t^4}{170001114}\\
&\quad-\frac{234833717t^5}{340002228}+\frac{17849899t^6}{170001114}-\frac{512491t^7}{85000557}, \qquad (43)\\
\alpha_{6,3}(t) &= -\frac{84921939t}{28333519}+\frac{341822079t^2}{113334076}+\frac{212325401t^3}{113334076}-\frac{962866223t^4}{340002228}\\
&\quad+\frac{378275309t^5}{340002228}-\frac{31300007t^6}{170001114}+\frac{952939t^7}{85000557}, \qquad (44)\\
\alpha_{6,4}(t) &= \frac{69077727t}{28333519}-\frac{323751749t^2}{113334076}-\frac{7670551471t^3}{6120040104}+\frac{674853809t^4}{255001671}\\
&\quad-\frac{7166970445t^5}{6120040104}+\frac{214350505t^6}{1020006684}-\frac{20816779t^7}{1530010026}, \qquad (45)\\
\alpha_{6,5}(t) &= -\frac{575349399t}{566670380}+\frac{1417489173t^2}{1133340760}+\frac{530504683t^3}{1133340760}-\frac{781502957t^4}{680004456}\\
&\quad+\frac{1837449149t^5}{3400022280}-\frac{172476367t^6}{1700011140}+\frac{5783299t^7}{850005570}, \qquad (46)\\
\alpha_{6,6}(t) &= 1, \qquad (47)\\
\beta_{6,\frac{11}{2}}(t) &= \frac{10988800t}{28333519}-\frac{13976256t^2}{28333519}-\frac{41612704t^3}{255001671}+\frac{38224480t^4}{85000557}\\
&\quad-\frac{56509600t^5}{255001671}+\frac{3704288t^6}{85000557}-\frac{776896t^7}{255001671}, \qquad (48)\\
\gamma_{6,\frac{11}{2}}(t) &= -\frac{3970368t}{28333519}+\frac{5134256t^2}{28333519}+\frac{4737112t^3}{85000557}-\frac{4656440t^4}{28333519}\\
&\quad+\frac{7069864t^5}{85000557}-\frac{477816t^6}{28333519}+\frac{104128t^7}{85000557}. \qquad (49)
\end{aligned}$$

putting $t=5$, into (41)–(49) lead to the following discrete coefficients

$$\alpha_{6,0}(5)=-\tfrac{139099}{28333519},\quad \alpha_{6,1}(5)=\tfrac{3692882}{85000557},\quad \alpha_{6,2}(5)=-\tfrac{4984665}{28333519}, \qquad (50)$$

$$\alpha_{6,3}(5)=\tfrac{12544580}{28333519},\quad \alpha_{6,4}(5)=-\tfrac{71374295}{85000557},\quad \alpha_{6,5}(5)=\tfrac{43473174}{28333519}, \qquad (51)$$

$$\alpha_{6,6}(5)=1,\quad \beta_{6,\frac{11}{2}}(5)=\tfrac{18905600}{28333519},\quad \gamma_{6,\frac{11}{2}}(5)=\tfrac{5842560}{28333519}. \qquad (52)$$

Also, for method of order 8 of (4) for $k=7$, we have

$$\begin{aligned}\alpha_{7,0}(t) &= -\frac{922103611t}{7640285694} + \frac{1457048238 47t^2}{458417141640} - \frac{299359941161t^3}{916834283280} \\ &\quad + \frac{9925284401t^4}{57302142705} - \frac{9531364111t^5}{183366856656} + \frac{8174610011t^6}{916834283280} \\ &\quad - \frac{186986651t^7}{229208570820} + \frac{28333519t^8}{916834283280},\end{aligned} \tag{53}$$

$$\begin{aligned}\alpha_{7,1}(t) &= 1 - \frac{124803885833t}{76402856940} + \frac{10965552103t^2}{152805713880} + \frac{3234973343t^3}{2546761898} \\ &\quad - \frac{51159414733t^4}{50935237960} + \frac{9085978741t^5}{25467618980} - \frac{3417969021t^6}{50935237960} \\ &\quad + \frac{24837466t^7}{3820142847} - \frac{39114721t^8}{152805713880},\end{aligned} \tag{54}$$

$$\begin{aligned}\alpha_{7,2}(t) &= \frac{84190027955t}{22920857082} - \frac{639918974387t^2}{275050284984} - \frac{126122591083t^3}{61122285552} \\ &\quad + \frac{59643199577t^4}{22920857082} - \frac{66421321777t^5}{61122285552} + \frac{40978157657t^6}{183366856656} \\ &\quad - \frac{1051264183t^7}{45841714164} + \frac{516970939t^8}{550100569968},\end{aligned} \tag{55}$$

$$\begin{aligned}\alpha_{7,3}(t) &= -\frac{15056659805t}{3820142847} + \frac{204757172807t^2}{45841714164} + \frac{22368750080t^3}{11460428541} \\ &\quad - \frac{184758894275t^4}{45841714164} + \frac{22260642617t^5}{11460428541} - \frac{19905894863t^6}{45841714164} \\ &\quad + \frac{540586718t^7}{11460428541} - \frac{92383669t^8}{45841714164},\end{aligned} \tag{56}$$

$$\begin{aligned}\alpha_{7,4}(t) &= \frac{28075810895t}{7640285694} - \frac{145953554021t^2}{30561142776} - \frac{27118376311t^3}{20374095184} \\ &\quad + \frac{10756657019t^4}{2546761898} - \frac{46465345373t^5}{20374095184} + \frac{11191778393t^6}{20374095184} \\ &\quad - \frac{963830527t^7}{15280571388} + \frac{172004407t^8}{61122285552},\end{aligned} \tag{57}$$

$$\begin{aligned}\alpha_{7,5}(t) &= -\frac{123634560709t}{45841714164} + \frac{5126517504559t^2}{1375251424920} + \frac{28405051519t^3}{38201428470} \\ &\quad - \frac{1484898234133t^4}{458417141640} + \frac{28951278721t^5}{15280571388} - \frac{222683878133t^6}{458417141640} \\ &\quad + \frac{3368328404t^7}{57302142705} - \frac{3771167761t^8}{1375251424920},\end{aligned} \tag{58}$$

$$\begin{aligned}\alpha_{7,6}(t) &= \frac{39912091879t}{38201428470} - \frac{679177442119t^2}{458417141640} - \frac{44857180987t^3}{183366856656} \\ &+ \frac{73057172414t^4}{57302142705} - \frac{710106178301t^5}{916834283280} + \frac{188313669923t^6}{916834283280} \\ &- \frac{1174906093t^7}{45841714164} + \frac{1126455691t^8}{916834283280},\end{aligned} \tag{59}$$

$$\alpha_{7,7}(t) = 1, \tag{60}$$

$$\begin{aligned}\beta_{7,\frac{13}{2}}(t) &= -\frac{1417502720t}{3820142847} + \frac{6138336512t^2}{11460428541} + \frac{958392 96t^3}{1273380949} \\ &- \frac{1746438176t^4}{3820142847} + \frac{363896960t^5}{1273380949} - \frac{297782464t^6}{3820142847} \\ &+ \frac{38293952t^7}{3820142847} - \frac{5674592t^8}{11460428541},\end{aligned} \tag{61}$$

$$\begin{aligned}\gamma_{7,\frac{13}{2}}(t) &= \frac{162208640t}{1273380949} - \frac{709049504t^2}{3820142847} - \frac{30068192t^3}{1273380949} \\ &+ \frac{200751096t^4}{1273380949} - \frac{127500800t^5}{1273380949} + \frac{35363888t^6}{1273380949} \\ &- \frac{4639648t^7}{1273380949} + \frac{704552t^8}{3820142847},\end{aligned} \tag{62}$$

Putting $t = 6$ into (53)–(62) give the discrete coefficients of (4) of order 8 as,

$$\alpha_{7,0}(6) = \tfrac{4447381}{1273380949}, \quad \alpha_{7,1}(6) = -\tfrac{43089403}{1273380949}, \quad \alpha_{7,2}(6) = \tfrac{571700227}{3820142847}, \tag{63}$$

$$\alpha_{7,3}(6) = -\tfrac{514044335}{1273380949}, \quad \alpha_{7,4}(6) = \tfrac{968766575}{1273380949}, \quad \alpha_{7,5}(6) = -\tfrac{4391629123}{3820142847}, \tag{64}$$

$$\alpha_{7,6}(6) = \tfrac{2130610363}{1273380949}, \ \alpha_{7,7}(6) = 1, \ \beta_{7,\frac{13}{2}}(6) = \tfrac{778408960}{1273380949}, \ \gamma_{7,\frac{13}{2}}(6) = \tfrac{289121280}{1273380949}. \tag{65}$$

3 The derivation of the continuous hybrid predictor

Similarly, the corresponding hybrid predictor

$$y(x_n + vh) = \sum_{j=0}^{k} \alpha_j(t) y_{n+j} + h\phi_k(t) f_{n+k}, \quad v = t+1, \ t = k - 3/2 \tag{66}$$

for $f(x_{n+v})$ in (2) are obtained from the polynomial interpolant

$$y(x_{n+v}) = \sum_{j=0}^{k+1} b_j x^j. \tag{67}$$

where $\{b\}_{j=0}^{k+1}$ are the real parameter constants to be determined. Following the same procedure in section 2, the unknown continuous coefficients of the hybrid predictors in (5) are obtained. After some simplifications, we obtained a class of continuous hybrid predictors from (5). Below is the continuous and the discrete coefficients of the predictor (5) for $k \le 7$. For example, if we set $k = 1$ and $t = k - \frac{3}{2}$, in (5) we obtain

$$\alpha_0(t) = t^2, \quad \alpha_{\frac{1}{2}}(t) = 1, \quad \alpha_1(t) = 1 - t^2, \quad \phi_1(t) = t + t^2. \tag{68}$$

Substituting $t = -\frac{1}{2}$ into (68) give the discrete coefficient values

$$\alpha_0\left(-\frac{1}{2}\right) = \frac{1}{4}, \ \ \alpha_{\frac{1}{2}}\left(-\frac{1}{2}\right) = 1, \ \ \alpha_1\left(-\frac{1}{2}\right) = \frac{3}{4}, \ \ \phi_1\left(-\frac{1}{2}\right) = -\frac{1}{4}, \tag{69}$$

of the hybrid predictor in (3). For $k = 2$ in (5) yield the following continuous coefficients

$$\alpha_0(t) = -\frac{t}{4} + \frac{t^2}{2} - \frac{t^3}{4}, \quad \alpha_1(t) = 1 - t - t^2 + t^3, \tag{70}$$

$$\alpha_{\frac{3}{2}}(t) = 1, \quad \alpha_2(t) = \frac{5t}{4} + \frac{t^2}{2} - \frac{3t^3}{4}, \quad \phi_2(t) = -\frac{t}{2} + \frac{t^3}{2}. \tag{71}$$

Inserting $t = \frac{1}{2}$ into (70) and (71) we obtained

$$\alpha_0\left(\tfrac{1}{2}\right) = -\tfrac{1}{32}, \ \ \alpha_1\left(\tfrac{1}{2}\right) = \tfrac{12}{32}, \ \ \alpha_{\frac{3}{2}}\left(\tfrac{1}{2}\right) = 1, \ \ \alpha_2\left(\tfrac{1}{2}\right) = \tfrac{21}{32}, \ \ \phi_2\left(\tfrac{1}{2}\right) = -\tfrac{6}{32}. \tag{72}$$

Again, fixing $k = 3$ in (5) yield,

$$\begin{gathered} \alpha_0(t) = -\frac{2t}{9} + \frac{4t^2}{9} - \frac{5t^3}{18} + \frac{t^4}{18}, \\ \alpha_1(t) = 1 - t - \tfrac{3t^2}{4} + t^3 - \tfrac{t^4}{4}, \\ \alpha_2(t) = 2t - \frac{3t^3}{2} + \frac{t^4}{2}, \quad \alpha_{\frac{5}{2}}(t) = 1, \\ \alpha_3(t) = -\frac{7t}{9} + \frac{11t^2}{36} + \frac{7t^3}{9} - \frac{11t^4}{36}, \end{gathered} \tag{73}$$

$$\phi_3(t) = \frac{t}{3} - \frac{t^2}{6} - \frac{t^3}{3} + \frac{t^4}{6}, \tag{74}$$

replacing t with $\frac{3}{2}$ in (73) and (74), lead to

$$\begin{gathered} \alpha_0\left(\tfrac{3}{2}\right) = \tfrac{1}{96}, \quad \alpha_1\left(\tfrac{3}{2}\right) = -\tfrac{5}{64}, \quad \alpha_2\left(\tfrac{3}{2}\right) = \tfrac{15}{32}, \quad \alpha_{\frac{5}{2}}\left(\tfrac{3}{2}\right) = 1, \\ \alpha_3\left(\tfrac{3}{2}\right) = \tfrac{115}{192}, \quad \phi_3\left(\tfrac{3}{2}\right) = -\tfrac{5}{32}. \end{gathered} \tag{75}$$

The order of the algorithm in (5) for $k = 3$ is 4. Putting $k = 4$ in (5), we have the hybrid solution scheme of order 5 continuous coefficients:

$$\alpha_0(t) = -\frac{3t}{16} + \frac{13t^2}{32} - \frac{29t^3}{96} + \frac{3t^4}{32} - \frac{t^5}{96}, \tag{76}$$

$$\alpha_1(t) = 1 - \frac{7t}{6} - \frac{5t^2}{9} + \frac{10t^3}{9} - \frac{4t^4}{9} + \frac{t^5}{18}, \tag{77}$$

$$\alpha_2(t) = \frac{9t}{4} - \frac{3t^2}{8} - \frac{13t^3}{8} + \frac{7t^4}{8} - \frac{t^5}{8}, \tag{78}$$

$$\alpha_3(t) = -\frac{3t}{2} + t^2 + \frac{4t^3}{3} - t^4 + \frac{t^5}{6}, \quad \alpha_{\frac{7}{2}}(t) = 1, \tag{79}$$

$$\alpha_4(t) = \frac{29t}{48} - \frac{137t^2}{288} - \frac{149t^3}{288} + \frac{137t^4}{288} - \frac{25t^5}{288}, \tag{80}$$

$$\phi_4(t) = -\frac{t}{4} + \frac{5t^2}{24} + \frac{5t^3}{24} - \frac{5t^4}{24} + \frac{t^5}{24}, \tag{81}$$

setting $t = \frac{5}{2}$ in (76)–(81) with a tedious simplification, we obtain

$$\alpha_0(\tfrac{5}{2}) = -\tfrac{5}{1024}, \quad \alpha_1(\tfrac{5}{2}) = \tfrac{7}{192}, \quad \alpha_2(\tfrac{5}{2}) = -\tfrac{35}{256}, \tag{82}$$

$$\alpha_3(\tfrac{5}{2}) = \tfrac{35}{64}, \quad \alpha_{\frac{7}{2}}(\tfrac{5}{2}) = 1, \quad \alpha_4(\tfrac{5}{2}) = \tfrac{1715}{3072}, \quad \phi_4(\tfrac{5}{2}) = -\tfrac{35}{256}. \tag{83}$$

For $k = 5$ in (5), we found that the scheme in (5) of order 6 has coefficients as

$$\alpha_0(t) = -\frac{4t}{25} + \frac{28t^2}{75} - \frac{19t^3}{60} + \frac{t^4}{8} - \frac{7t^5}{300} + \frac{t^6}{600}, \tag{84}$$

$$\alpha_1(t) = 1 - \frac{4t}{3} - \frac{17t^2}{48} + \frac{115t^3}{96} - \frac{61t^4}{96} + \frac{13t^5}{96} - \frac{t^6}{96}, \tag{85}$$

$$\alpha_2(t) = \frac{8t}{3} - \frac{8t^2}{9} - \frac{11t^3}{6} + \frac{49t^4}{36} - \frac{t^5}{3} + \frac{t^6}{36}, \tag{86}$$

$$\alpha_3(t) = -2t + \frac{5t^2}{3} + \frac{37t^3}{24} - \frac{13t^4}{8} + \frac{11t^5}{24} - \frac{t^6}{24}, \tag{87}$$

$$\alpha_4(t) = \frac{4t}{3} - \frac{4t^2}{3} - \frac{11t^3}{12} + \frac{31t^4}{24} - \frac{5t^5}{12} + \frac{t^6}{24}, \tag{88}$$

$$\alpha_5(t) = -\frac{38t}{75} + \frac{1931t^2}{3600} + \frac{157t^3}{480} - \frac{149t^4}{288} + \frac{431t^5}{2400} - \frac{137t^6}{7200}, \tag{89}$$

$$\alpha_{\frac{9}{2}}(t) = 1, \quad \phi_5(t) = \frac{t}{5} - \frac{13t^2}{60} - \frac{t^3}{8} + \frac{5t^4}{24} - \frac{3t^5}{40} + \frac{t^6}{120}, \tag{90}$$

replacing t by $\frac{7}{2}$ in (84)–(90) lead to

$$\alpha_0(\tfrac{7}{2}) = \tfrac{7}{2560}, \quad \alpha_1(\tfrac{7}{2}) = -\tfrac{45}{2048}, \quad \alpha_2(\tfrac{7}{2}) = \tfrac{21}{256}, \quad \alpha_3(\tfrac{7}{2}) = -\tfrac{105}{512}, \tag{91}$$

$$\alpha_4(\tfrac{7}{2}) = \tfrac{315}{512}, \quad \alpha_5(\tfrac{7}{2}) = \tfrac{5397}{10240}, \quad \alpha_{\frac{9}{2}}(\tfrac{7}{2}) = 1, \quad \phi_5(\tfrac{7}{2}) = -\tfrac{63}{512}. \tag{92}$$

More so, fixing $k=6$ in (5) yield the following continuous coefficients

$$\alpha_0(t) = -\frac{5t}{36}+\frac{149t^2}{432}-\frac{1399t^3}{4320}+\frac{65t^4}{432}-\frac{t^5}{27}+\frac{t^6}{216}-\frac{t^7}{4320}, \quad (93)$$

$$\alpha_1(t) = 1-\frac{89t}{60}-\frac{91t^2}{600}+\frac{749t^3}{600}-\frac{49t^4}{60}+\frac{7t^5}{30}-\frac{19t^6}{600}+\frac{t^7}{600}, \quad (94)$$

$$\alpha_2(t) = \frac{25t}{8}-\frac{145t^2}{96}-\frac{127t^3}{64}+\frac{23t^4}{12}-\frac{61t^5}{96}+\frac{3t^6}{32}-\frac{t^7}{192}, \quad (95)$$

$$\alpha_3(t) = -\frac{25t}{9}+\frac{295t^2}{108}+\frac{193t^3}{108}-\frac{139t^4}{54}+\frac{53t^5}{54}-\frac{17t^6}{108}+\frac{t^7}{108}, \quad (96)$$

$$\alpha_4(t) = \frac{25t}{12}-\frac{115t^2}{48}-\frac{107t^3}{96}+\frac{107t^4}{48}-\frac{23t^5}{24}+\frac{t^6}{6}-\frac{t^7}{96}, \quad (97)$$

$$\alpha_5(t) = -\frac{5t}{4}+\frac{37t^2}{24}+\frac{23t^3}{40}-\frac{17t^4}{12}+\frac{2t^5}{3}-\frac{t^6}{8}+\frac{t^7}{120}, \quad (98)$$

$$\alpha_6(t) = \frac{53t}{120}-\frac{4033t^2}{7200}-\frac{2701t^3}{14400}+\frac{23t^4}{45}-\frac{361t^5}{1440}+\frac{353t^6}{7200}-\frac{49t^7}{14400}, \quad (99)$$

$$\alpha_{\frac{11}{2}}(t) = 1, \quad \phi_6(t) = -\frac{t}{6}+\frac{77t^2}{360}+\frac{49t^3}{720}-\frac{7t^4}{36}+\frac{7t^5}{72}-\frac{7t^6}{360}+\frac{t^7}{720} \quad (100)$$

of method of order 7. Substituting $t=\frac{9}{2}$ into (93)–(100) yields

$$\alpha_0(\tfrac{9}{2}) = -\tfrac{7}{4096}, \quad \alpha_1(\tfrac{9}{2}) = \tfrac{77}{5120}, \quad \alpha_2(\tfrac{9}{2}) = -\tfrac{495}{8192}, \quad \alpha_3(\tfrac{9}{2}) = \tfrac{77}{512}, \quad (101)$$

$$\alpha_4(\tfrac{9}{2}) = -\tfrac{1155}{4096}, \quad \alpha_5(\tfrac{9}{2}) = \tfrac{693}{1024}, \quad \alpha_{\frac{11}{2}}(\tfrac{9}{2}) = 1, \quad \phi_6(\tfrac{9}{2}) = -\tfrac{231}{2048}. \quad (102)$$

Fixing $k=7$ in (5) we obtain:

$$\alpha_0(t) = -\frac{6t}{49}+\frac{157t^2}{490}-\frac{137t^3}{420}+\frac{431t^4}{2520}-\frac{17t^5}{336}+\frac{43t^6}{5040} -\frac{3t^7}{3920}+\frac{t^8}{35280}, \quad (103)$$

$$\alpha_1(t) = 1-\frac{97t}{60}+\frac{17t^2}{360}+\frac{2737t^3}{2160}-\frac{4249t^4}{4320}+\frac{371t^5}{1080}-\frac{137t^6}{2160} +\frac{13t^7}{2160}-\frac{t^8}{4320}, \quad (104)$$

$$\alpha_2(t) = \frac{18t}{5}-\frac{111t^2}{50}-\frac{41t^3}{20}+\frac{1507t^4}{600}-\frac{247t^5}{240}+\frac{83t^6}{400}-\frac{t^7}{48}+\frac{t^8}{1200}, \quad (105)$$

$$\alpha_3(t) = -\frac{15t}{4}+\frac{67t^2}{16}+\frac{23t^3}{12}-\frac{2185t^4}{576}+\frac{43t^5}{24}-\frac{113t^6}{288}+\frac{t^7}{24}-\frac{t^8}{576}, \quad (106)$$

$$\alpha_4(t) = \frac{10t}{3} - \frac{77t^2}{18} - \frac{137t^3}{108} + \frac{821t^4}{216} - \frac{869t^5}{432} + \frac{205t^6}{432} - \frac{23t^7}{432} + \frac{t^8}{432}, \quad (107)$$

$$\alpha_5(t) = -\frac{9t}{4} + \frac{123t^2}{40} + \frac{53t^3}{80} - \frac{1289t^4}{480} + \frac{37t^5}{24} - \frac{31t^6}{80} + \frac{11t^7}{240} - \frac{t^8}{480}, \quad (108)$$

$$\alpha_6(t) = \frac{6t}{5} - \frac{17t^2}{10} - \frac{17t^3}{60} + \frac{527t^4}{360} - \frac{71t^5}{80} + \frac{169t^6}{720} - \frac{7t^7}{240} + \frac{t^8}{720}, \quad (109)$$

$$\alpha_{\frac{13}{2}}(t) = 1, \quad (110)$$

$$\alpha_7(t) = -\frac{1159t}{2940} + \frac{100133t^2}{176400} + \frac{103t^3}{1260} - \frac{48901t^4}{100800} + \frac{761t^5}{2520} - \frac{4133t^6}{50400} + \frac{37t^7}{3528} - \frac{121t^8}{235200}, \quad (111)$$

$$\phi_7(t) = \frac{t}{7} - \frac{29t^2}{140} - \frac{t^3}{36} + \frac{127t^4}{720} - \frac{t^5}{9} + \frac{11t^6}{360} - \frac{t^7}{252} + \frac{t^8}{5040} \quad (112)$$

inserting $t = \frac{11}{2}$ into (103)–(112) result to

$$\alpha_0(\tfrac{11}{2}) = \tfrac{33}{28672}, \quad \alpha_1(\tfrac{11}{2}) = -\tfrac{91}{8192}, \quad \alpha_2(\tfrac{11}{2}) = \tfrac{1001}{20480}, \quad (113)$$

$$\alpha_3(\tfrac{11}{2}) = -\tfrac{2145}{16384}, \quad \alpha_4(\tfrac{11}{2}) = \tfrac{1001}{4096}, \quad \alpha_5(\tfrac{11}{2}) = -\tfrac{3003}{8192}, \quad (114)$$

$$\alpha_6(\tfrac{11}{2}) = \tfrac{3003}{4096}, \quad \alpha_7(\tfrac{11}{2}) = \tfrac{275847}{573440}, \quad \alpha_{\frac{13}{2}}(\tfrac{11}{2}) = 1, \quad \phi_7(\tfrac{11}{2}) = -\tfrac{429}{4096}. \quad (115)$$

Expanding and simplifying (8) and (9) by Taylor's series respectively, we obtained the error constants and order of the schemes in the tables below. Table 1 show the step number, the continuous and the discrete versions of the error constants of the scheme (4). Table 2 show the step number, the continuous and the discrete versions of the error constants of (5). C_{p+1} and C^*_{p+1} in Table 1 and Table 2 implies discrete error constants for the MSD-BDF (4) and hybrid predictor (5) respectively.

4 The boundary locus of the discrete MSD-BDF

In this section the stability properties of the proposed method (4) is carried out to show its suitability for stiff IVPs (3). This method can only be suitable as integrators for (3) if it is zero stable and more importantly for stiff ODE it must be A-stable or stiffly stable. On substituting the discrete version of the hybrid predictor (5) in (4) for a corresponding k and applying the resultant scheme to the scalar test problem $y' = \lambda y$, $\mathrm{Re}(\lambda) < 0$, we obtain a quadratic polynomial that takes the form

$$\pi(r,z) = r^k - \sum_{j=0}^{k-1} r^j \alpha_{k,j} - z\beta_{k,v}\left(\sum_{j=0}^{k} r^j \alpha_j + r^k z\phi_k\right) - z^2\gamma_{k,v}\left(\sum_{j=0}^{k} r^j \alpha_j + r^k z\phi_k\right) = 0, \quad z = \lambda h. \quad (116)$$

Table 1 The Continuous and Discrete Error Constants of Method (4).

k	t	Continuous Error Constant $(C_{p+1}(t))$	C_{p+1}
1	0	$\frac{(1+t)\left(1+2t+4t^2\right)}{24}h^3y^{(3)}(x_n)$	$\frac{1}{24}$
2	1	$\frac{t(1+t)\left(17-38t+26t^2\right)}{624}h^4y^{(4)}(x_n)$	$\frac{5}{312}$
3	2	$\frac{(-1+t)t(1+t)(2403+t(-2709+788t))}{94560}h^5y^{(5)}(x_n)$	$\frac{137}{15760}$
4	3	$\frac{(-2+t)(-1+t)t(1+t)(652075+8t(-59485+10973t))}{63204480}h^6y^{(6)}(x_n)$	$\frac{14491}{2633520}$
5	4	$\frac{(-3+t)(-2+t)(-1+t)t(1+t)\left(11984371-6436822t+868876t^2\right)}{4379135040}h^7y^{(7)}(x_n)$	$\frac{139099}{36492792}$
6	5	$\frac{(-4+t)(-3+t)(-2+t)(-1+t)t(1+t)(627493311+t(-266276781+28333519t))}{1142407486080}h^8y^{(8)}(x_n)$	$\frac{4447381}{1586677064}$
7	6	$\frac{(-5+t)(-4+t)(-3+t)(-2+t)(-1+t)t(1+t)(330991590248+t(-116024591617+10187047592t))}{3696675830184960}h^9y^{(9)}(x_n)$	$\frac{788876929}{366733713312}$

Table 2 The Continuous and Discrete Error Constants of Predictor (5)

k	t	Continuous Error Constant ($C^*_{p+1}(t)$)	C^*_{p+1}
1	$\frac{-1}{2}$	$\frac{1}{6}t^2(1+t)h^3y^{(3)}(x_n)$	$\frac{1}{48}$
2	$\frac{1}{2}$	$\frac{1}{24}(-1+t)^2t(1+t)h^4y^{(4)}(x_n)$	$\frac{1}{128}$
3	$\frac{3}{2}$	$\frac{1}{120}(-2+t)^2t(-1+t^2)h^5y^{(5)}(x_n)$	$\frac{1}{256}$
4	$\frac{5}{2}$	$\frac{1}{720}(-3+t)^2(-2+t)(-1+t)t(1+t)h^6y^{(6)}(x_n)$	$\frac{7}{3072}$
5	$\frac{7}{2}$	$\frac{1}{5040}(-4+t)^2(-3+t)(-2+t)(-1+t)t(1+t)h^7y^{(7)}(x_n)$	$\frac{3}{2048}$
6	$\frac{9}{2}$	$\frac{1}{40320}(-5+t)^2(-4+t)(-3+t)(-2+t)(-1+t)t(1+t)h^8y^{(8)}(x_n)$	$\frac{33}{32768}$
7	$\frac{11}{2}$	$\frac{1}{362880}(-6+t)^2(-5+t)(-4+t)(-3+t)(-2+t)(-1+t)t(1+t)h^9y^{(9)}(x_n)$	$\frac{143}{196608}$

Let $\rho(r)$ denotes the first characteristics polynomial of $\pi(r,z)$for $k \leq 7$, method (4) is said to be zero stable if the roots of $\rho(r)=0$ are inside the unit disk with simple roots on the unit disk. If the absolute value of the roots of $\pi(r,z)$ lies on the entire left half of the z complex plane, then method (4) is said to be A-stable. Also, method (4) is said to be $A(\alpha)$ stable for some $\alpha \in [0, \frac{\pi}{2}]$ if the wedge $S_\alpha=\{z\colon |Arg(-z)| < \alpha, z \neq 0\}$ is contained in its region of absolute stability. See Fig. 1(a). The largest $\alpha(\alpha_{\max})$ is regarded as the angle of absolute stability on the argument of stability. The definition of stiff stability in the spirit of Gear in [18, 19] show that stiff stability implies $A(\alpha)$-stability. Also see [16], [21] and [32].

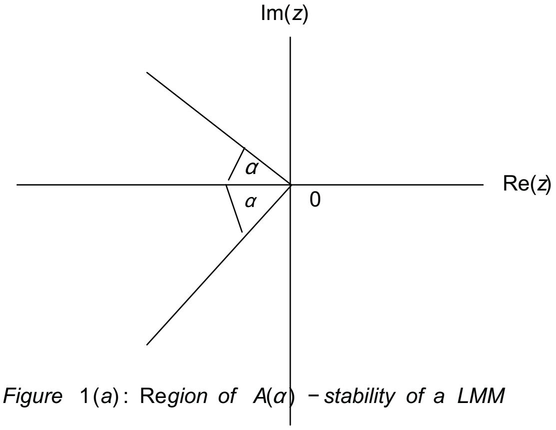

Figure 1(a): Region of A(α) − stability of a LMM

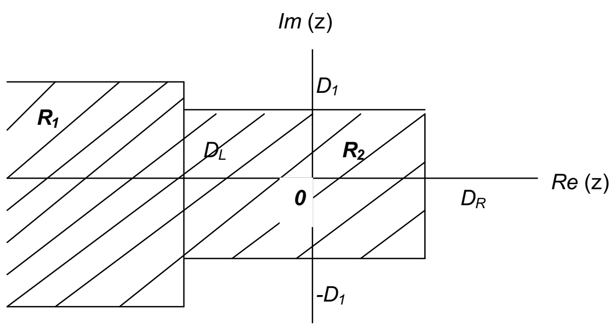

Figure 1(b): Region of stiff-stability of a LMM

Figure 1: The diagrams of region of $A(\alpha)$ and stiff stabilities of a LMM.

4.1 Methods with large intervals of absolute stability on z complex plane

In this subsection we give pair of the discrete scheme ((4) and (5)) and their respective stability functions whose continuous and discrete coefficients have been derived in section 2 and 3 respectively for a fixed values of k and t. Consider the first method of order $p = 2$ (i.e. $k = 1$) defined in ((4) and (5)),

$$y_{n+\frac{1}{2}} = \frac{1}{4}y_n + \frac{3}{4}y_{n+1} - \frac{h}{4}f_{n+1}, \tag{117}$$

$$y_{n+1} = y_n + hf_{n+\frac{1}{2}}, \tag{118}$$

has stability function

$$\pi_1(r,z) = r - 1 - \frac{z}{4} - \frac{3rz}{4} + \frac{rz^2}{4}.$$

The method in (117) and (118) is a typical example of an implicit one-leg LMM type, such have been discussed in the works of [2], [16], and [21] respectively. Setting $z = 0$ in the stability polynomial $\pi_1(r,z)$ we verify that the root(s), (r_j) of the first characteristics polynomial has $|r_j| \leq 1$, which obviously implies zero stability. We have plotted in Fig. 1 the boundary of the stability region of $\pi_1(r,z)$ and found that interval of absolute stability of the scheme ((4) and (5)) is $(-\infty, 0)$ which implies that the angle (α) of absolute stability of the algorithm ((4) and (5)) is $90°$. Consider next the method ((4) and (5)) of order three respectively,

$$y_{n+\frac{3}{2}} = -\frac{1}{32}y_n + \frac{12}{32}y_{n+1} + \frac{21}{32}y_{n+2} - \frac{6}{32}hf_{n+2} \tag{119}$$

$$y_{n+2} = -\frac{1}{13}y_n + \frac{14}{13}y_{n+1} + \frac{12}{13}hf_{n+\frac{3}{2}} + \frac{h^2}{13}f'_{n+\frac{3}{2}}, \tag{120}$$

whose stability polynomial is

$$\pi_2(r,z) = \frac{1}{13} - \frac{14r}{13} + r^2 + \frac{3z}{104} - \frac{9rz}{26} - \frac{63r^2z}{104} + \frac{z^2}{416} - \frac{3rz^2}{104} + \frac{51r^2z^2}{416} + \frac{3r^2z^3}{208}.$$

With $z = 0$ in $\pi_2(r,z)$, thus the first characteristics polynomial $\pi_2(r,0) = 0$ yields roots: $r_1 = \frac{1}{13}$ and $r_2 = 1$, with $|r_{1,2}| \leq 1$, implying zero stability of (119) and (120). The stability plot in Fig. 2 in boundary locus sense revealed that the scheme in (119) and (120) is stable in the entire left half of the z complex plane, which shows that the method is A-stable, $(\alpha = 90°)$. Therefore, the interval of absolute stability of ((4) and (5)) is $(-\infty, 0)$ for $k = 2$. Again, we consider another method

$$y_{n+\frac{5}{2}} = \frac{1}{96}y_n - \frac{5}{64}y_{n+1} + \frac{15}{32}y_{n+2} + \frac{115}{192}y_{n+3} - \frac{5}{32}hf_{n+3} \tag{121}$$

$$y_{n+3} = \frac{5}{197}y_n - \frac{39}{197}y_{1+n} + \frac{231}{197}y_{2+n} + \frac{168}{197}hf_{n+\frac{5}{2}} + \frac{24}{197}h^2f'_{n+\frac{5}{2}} \tag{122}$$

of order four. Interestingly, the stability polynomial $\pi_3(r,z)$ of (121) and (122) which is a subset of ((2) and (3)) appearing in (116) takes the form

$$\pi_3(r,z) = -\frac{5}{197} + \frac{39r}{197} - \frac{231r^2}{197} + r^3 - \frac{7z}{788} + \frac{105rz}{1576} - \frac{315r^2z}{788} - \frac{805r^3z}{1576} - \frac{z^2}{788} + \frac{15rz^2}{1576} - \frac{45r^2z^2}{788} + \frac{95r^3z^2}{1576} + \frac{15r^3z^3}{788}. \quad (123)$$

The roots: $r_1 = 1$, and $r_{2,3} = \frac{1}{197}\left(17 \pm 2i\sqrt{174}\right)$ of the first characteristics polynomial of $\pi_3(r,0)$ are observed to have $|r_{1,2,3}| \le 1$, satisfying the condition of zero stability. The boundary of the stability region shows that the scheme ((4) and (5)) for $k = 3$ is stable at infinity, at the negative z complex plane. The line labeled $k = 3$ in Fig. 2 is the locus of the roots of $\pi_3(r,z)$. Thus, the interval of absolute stability is $(-\infty, 0)$. The measure of α show that $\alpha = 90°$. Therefore a new A-stable method is found.

For method of order five,

$$y_{n+\frac{7}{2}} = -\frac{5}{1024}y_n + \frac{7}{192}y_{n+1} - \frac{35}{256}y_{n+2} + \frac{35}{64}y_{n+3} + \frac{1715}{3072}y_{n+4} - \frac{35}{256}hf_{n+4}, \quad (124)$$

$$y_{n+4} = -\frac{137}{10973}y_n + \frac{1040}{10973}y_{n+1} - \frac{4002}{10973}y_{n+2} + \frac{14072}{10973}y_{n+3} + \frac{8640}{10973}hf_{n+\frac{7}{2}} + \frac{1704}{10973}h^2f'_{n+\frac{7}{2}}, \quad (125)$$

we obtained the stability function from (116) as

$$\pi_4(r,z) = \frac{137}{10973} - \frac{1040r}{10973} + \frac{4002r^2}{10973} - \frac{14072r^3}{10973} + r^4 + \frac{675z}{175568} - \frac{315rz}{10973} + \frac{4725r^2z}{43892} - \frac{4725r^3z}{10973} - \frac{77175r^4z}{175568} + \frac{1065z^2}{1404544} - \frac{497rz^2}{87784} + \frac{7455r^2z^2}{351136} - \frac{7455r^3z^2}{87784} + \frac{29435r^4z^2}{1404544} + \frac{7455r^4z^3}{351136} \quad (126)$$

The roots, $r_{1,2,3,4}$ of the first characteristics polynomial $\pi_4(r,0)$ are: 1, 0.19221556288702765, $0.0451025 + 0.250838i$, $0.0451025 - 0.250838i$, we verify that $|r_{1,2,3,4}| \le 1$. The boundary of the stability region of (126) labeled $k = 4$ is slight outside the positive imaginary of the z complex plane, hence the method is not A-stable. Therefore, the method is stiffly stable with an angle (α) of 87^0. Again, we investigate the stability property of method of order six of (4) and (5) for $k = 5$,

$$
\begin{aligned}
y_{n+\frac{9}{2}} &= \frac{7}{2560}y_n - \frac{45}{2048}y_{n+1} + \frac{21}{256}y_{n+2} - \frac{105}{512}y_{n+3} \\
&\quad + \frac{315}{512}y_{n+4} + \frac{5397}{10240}y_{n+5} - \frac{63}{512}hf_{n+5}, \qquad (127)\\
y_{n+5} &= \frac{14491}{1954971}y_n - \frac{13055}{217219}y_{n+1} + \frac{49390}{217219}y_{n+2} - \frac{1130590}{1954971}y_{n+3} \\
&\quad + \frac{304895}{217219}y_{n+4} + \frac{472960}{651657}hf_{n+\frac{9}{2}} + \frac{39680}{217219}h^2 f'_{n+\frac{9}{2}}. \qquad (128)
\end{aligned}
$$

Adopting the above procedure, the stability function of (129) is nicely obtained from (116) as

$$
\begin{aligned}
\pi_5(r,z) &= -\frac{14491}{1954971} + \frac{13055r}{217219} - \frac{49390r^2}{217219} + \frac{1130590r^3}{1954971} - \frac{304895r^4}{217219} + r^5 \\
&\quad - \frac{5173z}{2606628} + \frac{55425rz}{3475504} - \frac{25865r^2z}{434438} + \frac{129325r^3z}{868876} - \frac{387975r^4z}{868876} \\
&\quad - \frac{1329461r^5z}{3475504} - \frac{217z^2}{434438} + \frac{6975rz^2}{1737752} - \frac{3255r^2z^2}{217219} + \frac{16275r^3z^2}{434438} \\
&\quad - \frac{48825r^4z^2}{434438} - \frac{12117r^5z^2}{1737752} + \frac{9765r^5z^3}{434438}. \qquad (129)
\end{aligned}
$$

After a tedious computation, we found that the method in (4) for $k = 5$ is zero-stable with roots $r_{1,2,3,4,5} = 1,\ -0.0121366 + 0.3554i,\ -0.0121366 - 0.3554i,$ $0.213951 - 0.113318i$, $0.213951 + 0.113318i$ obtained from $\pi_5(r, 0)$ has

$$|r_{1,2,3,4,5}| \leq 1.$$

The angle of absolute stability of the algorithm (4) for $k = 5$ is $\alpha = 86°$. From the above definition, the scheme defined in (125) is observed to be stiffly stable. See the loci of the roots of $\pi_5(r, z)$ plotted in boundary locus sense which we have labeled $k = 5$ in Fig. 2. Consider again, method of order seven for $k = 6$,

$$
\begin{aligned}
y_{n+\frac{11}{2}} &= -\frac{7}{4096}y_n + \frac{77}{5120}y_{n+1} - \frac{495}{8192}y_{n+2} + \frac{77}{512}y_{n+3} - \frac{1155}{4096}y_{n+4} \\
&\quad + \frac{693}{1024}y_{n+5} + \frac{20559}{40960}y_{n+6} - \frac{231}{2048}hf_{n+6} \qquad (130)\\
y_{n+6} &= -\frac{139099}{28333519}y_n + \frac{3692882}{85000557}y_{n+1} - \frac{4984665}{28333519}y_{n+2} \\
&\quad + \frac{12544580}{28333519}y_{n+3} - \frac{71374295}{85000557}y_{n+4} + \frac{43473174}{28333519}y_{n+5} \\
&\quad + \frac{18905600}{28333519}hf_{n+\frac{11}{2}} + \frac{5842560}{28333519}h^2 f'_{n+\frac{11}{2}}, \qquad (131)
\end{aligned}
$$

which is derived from (2) has its stability function from (116) as

$$
\begin{aligned}
\pi_6(r,z) =& \frac{139099}{28333519} - \frac{3692882w}{85000557} + \frac{4984665r^2}{28333519} - \frac{12544580r^3}{28333519} \\
&+ \frac{71374295w^4}{85000557} - \frac{43473174r^5}{28333519} + r^6 + \frac{1582568575z}{436789528904} \\
&- \frac{3438271375rz}{109197382226} + \frac{27106088625r^2z}{218394764452} - \frac{16323767075r^3z}{54598691113} \\
&+ \frac{228589197375r^4z}{436789528904} - \frac{107872362675r^5z}{109197382226} + \frac{1956299055z^2}{1747158115616} \\
&- \frac{4250234175rz^2}{436789528904} + \frac{33507309825r^2z^2}{873579057808} - \frac{20178695955r^3z^2}{218394764452} \\
&+ \frac{282571534575r^4z^2}{1747158115616} - \frac{133346892195r^5z^2}{436789528904} - \frac{7847301000r^6z^2}{54598691113} \\
&+ \frac{29954925r^6z^3}{109197382226} + \frac{6032671425r^6z^4}{436789528904}, \qquad (132)
\end{aligned}
$$

for zero stability, the method in (4) for $k = 6$ has roots $r_{1,2,3,4,5,6}$=1, 0.26442, $-0.0765026+0.452362i$, $-0.0765026+0.452362i$, $0.211461-0.208548i$, $0.211461+0.208548i$, with $|r_{1,2,3,4,5,6}| \leq 1$. The angle of absolute stability of the scheme (4) for $k = 6$ is 82^0. Therefore, the method is stiffly stable. Finally, we investigate the stability properties of the method of order eight derived in section 2 and 3 for $k = 7$,

$$
\begin{aligned}
y_{n+\frac{13}{2}} =& \frac{33}{28672}y_n - \frac{91}{8192}y_{n+1} + \frac{1001}{20480}y_{n+2} - \frac{2145}{16384}y_{n+3} + \frac{1001}{4096}y_{n+4} \\
&- \frac{3003}{8192}y_{n+5} + \frac{3003}{4096}y_{n+6} + \frac{275847}{573440}y_{n+7} - \frac{429}{4096}hf_{n+7}, \qquad (133)
\end{aligned}
$$

$$
\begin{aligned}
y_{n+7} =& \frac{4447381}{1273380949}y_n - \frac{43089403}{1273380949}y_{n+1} + \frac{571700227}{3820142847}y_{n+2} \\
&- \frac{514044335}{1273380949}y_{n+3} + \frac{968766575}{1273380949}y_{n+4} - \frac{4391629123}{3820142847}y_{n+5} \\
&+ \frac{2130610363}{1273380949}y_{n+6} + \frac{778408960}{1273380949}hf_{n+\frac{13}{2}} + \frac{289121280}{1273380949}h^2f'_{n+\frac{13}{2}}, \qquad (134)
\end{aligned}
$$

from (116), the stability polynomial of method of order eight takes the form

$$
\begin{aligned}
\pi_7(r,z) =& -\frac{4447381}{1273380949} + \frac{43089403r}{1273380949} - \frac{571700227r^2}{3820142847} \\
&+ \frac{514044335r^3}{1273380949} - \frac{968766575r^4}{1273380949} + \frac{4391629123r^5}{3820142847} \\
&- \frac{2130610363r^6}{1273380949} + r^7 - \frac{3583635z}{5093523796} + \frac{69175015rz}{10187047592}
\end{aligned}
$$

$$- \frac{152185033r^2z}{5093523796} + \frac{1630553925r^3z}{20374095184} - \frac{760925165r^4z}{5093523796}$$
$$+ \frac{2282775495r^5z}{10187047592} - \frac{2282775495r^6z}{5093523796} - \frac{5991120993r^7z}{20374095184}$$
$$- \frac{1331055z^2}{5093523796} + \frac{25693395rz^2}{10187047592} - \frac{56525469r^2z^2}{5093523796}$$
$$+ \frac{605630025r^3z^2}{20374095184} - \frac{282627345r^4z^2}{5093523796} + \frac{847882035r^5z^2}{10187047592}$$
$$- \frac{847882035r^6z^2}{5093523796} - \frac{920814609r^7z^2}{20374095184} + \frac{121126005r^7z^3}{5093523796}. \quad (135)$$

The first characteristics polynomial $\pi(r, 0)$ of the stability function in (135) of $k = 7$ is zero stable with $|r_{1,2,3,4,5,6,7}| \leq 1$, where $r_{1,2,3,4,5,6,7} = 1$, $-0.14473 - 0.544342i$, $-0.14473 + 0.544342i$, $0.198838 - 0.292646i$, $0.198838 + 0.292646i$, $0.282487 - 0.090251i$, $0.282487 + 0.090251i$ are roots of $\pi(r, 0)$. The angle of absolute stability of the scheme of order eight is measured as $67°$. Hence, the method is stiffly stable.

The graph in Fig. 2 show the loci of (4) and (5) for $k \leq 7$. Interestingly, the methods are found to zero-stable for $k \leq 7$, for $k = 1, 2, 3$ the algorithm in (4) is observed to be A-stable and stiffly stable when $k = 4, 5, 6, 7$ respectively. The case of $k \geq 8$ are stiffly unstable. Our further research is to find good hybrid predictor that will improved the stability property of (1) than those we have reported in [30] and in this paper.

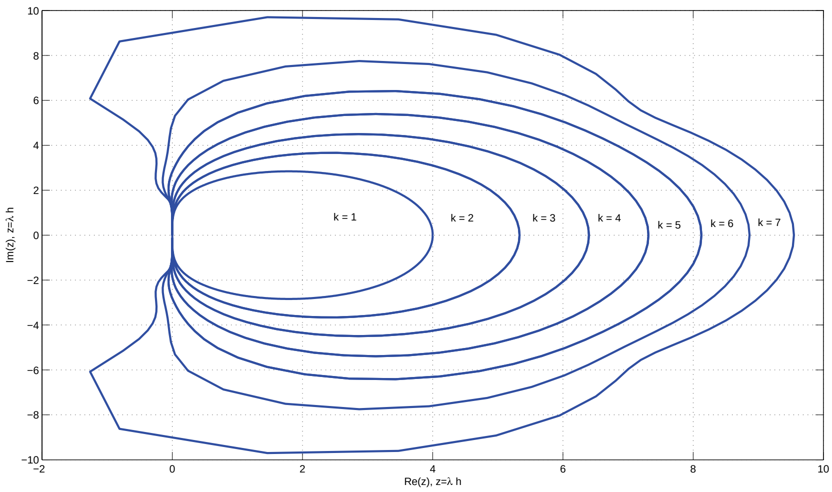

Figure 2: The boundary locus of the stability domain of the method (2) for $k \leq 7$. At $k = 8$, the loci of the method (2) was disconnected.

5 Numerical experiments

In this section we apply the discrete version of our proposed MSD-BDF of order 2

$$y_{n+\frac{1}{2}} = \frac{1}{4}y_n + \frac{3}{4}y_{n+1} - \frac{h}{4}f_{n+1}, \tag{136}$$

$$y_{n+1} = y_n + hf_{n+\frac{1}{2}}, \tag{137}$$

and *Ode15s code* of Matlab to the IVPs:
Prob. 1: A stiff system of Van der Pol equations discussed in [21]

$$y_1' = y_2, \quad y_2' = 1000(1-y_1^2)y_2 - y_1, \quad y(x) = \begin{pmatrix} 2 \\ 0 \end{pmatrix}, \quad x \in [0, 10],$$

Prob. 2: Nonlinear chemical problem in [13], [21] and [22]

$$\begin{cases} y_1' = -0.04y_1 + 10^4 y_2 y_3, & y_1(0) = 1, \\ y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3\times 10^7 y_2^2, & y_2(0) = 0, \\ y_3' = 3\times 10^7 y_2^2, & y_3(0) = 0, \\ x \in [0, 5], \quad h = 0.0001, & \end{cases}$$

The arising implicit set of nonlinear equations from the method on prob. 1 and 2 respectively is solved using the Newton Raphson iterative scheme,

$$y_{n+k}^{[s+1]} = y_{n+k}^{[s]} - F'(y_{n+k}^{[s]})^{-1}F(y_{n+k}^{[s]}), \quad s = 0, 1, 2, \dots \tag{138}$$

where,

$$y_{n+\frac{1}{2}}^{[s]} = \frac{1}{4}y_n + \frac{3}{4}y_{n+1}^{[s]} - \frac{h}{4}f(x_{n+1}, y_{n+1}^{[s]}), \tag{139}$$

$$F(y_{n+1}^{[s]}) = y_{n+1}^{[s]} - y_n - hf(x_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}^{[s]}), \tag{140}$$

and $F'(y_{n+1}^{[s]})^{-1}$ is the Jacobian matrix of the vector systems of the method. The starting value (i.e. $y_{n+1}^{[0]}$) for (138) is obtained from the trapezoidal rule

$$y_{n+1}^{[0]} = y_n + \frac{h}{2}(f_{n-1} + f_n), \quad s = 0, 1, 2, \dots \tag{141}$$

The numerical solution for method (4) and *Ode15s code* of Matlab of the first ($y_1(x)$) and second ($y_2(x)$) components for prob. 1 and prob. 2 respectively are given in the figures below:

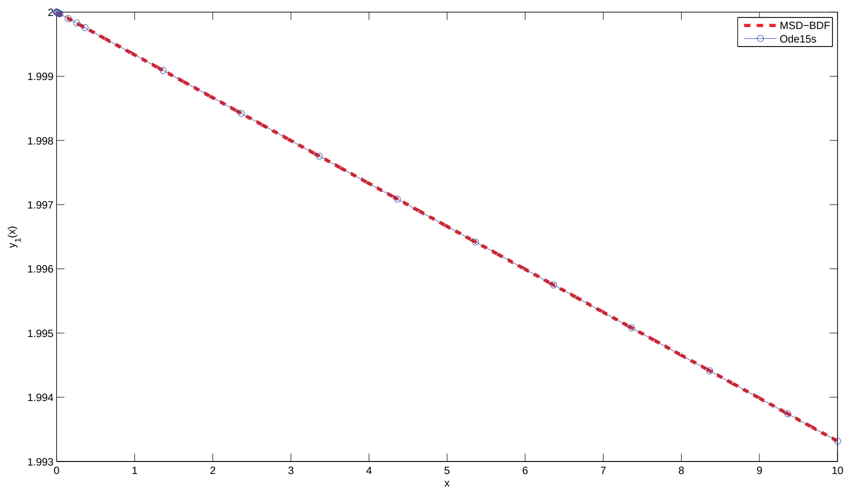

Figure 3: The plot of numerical solutions of $y_1(x)$ component of van der Pol's stiff IVPs in Prob. 1.

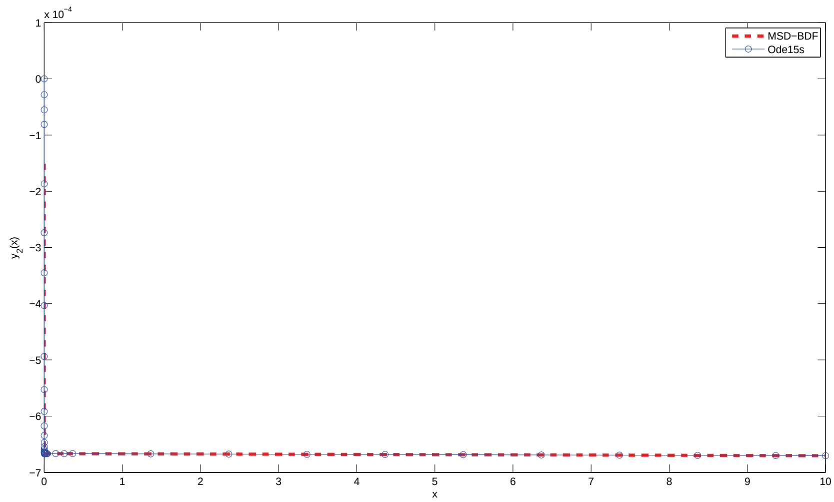

Figure 4: The plot of numerical solutions of $y_2(x)$ component of van der Pol's stiff IVPs in Prob. 1.

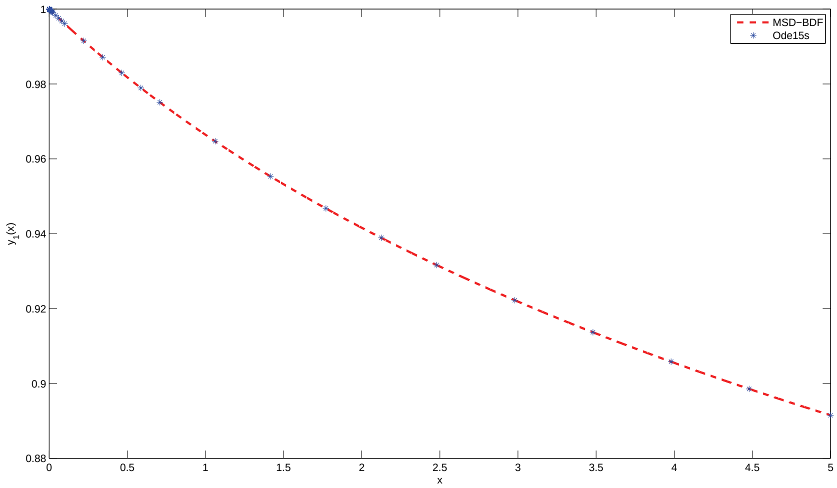

Figure 5: The plot of numerical solutions of $y_1(x)$ component of the nonlinear chemical stiff IVPs in Prob. 2.

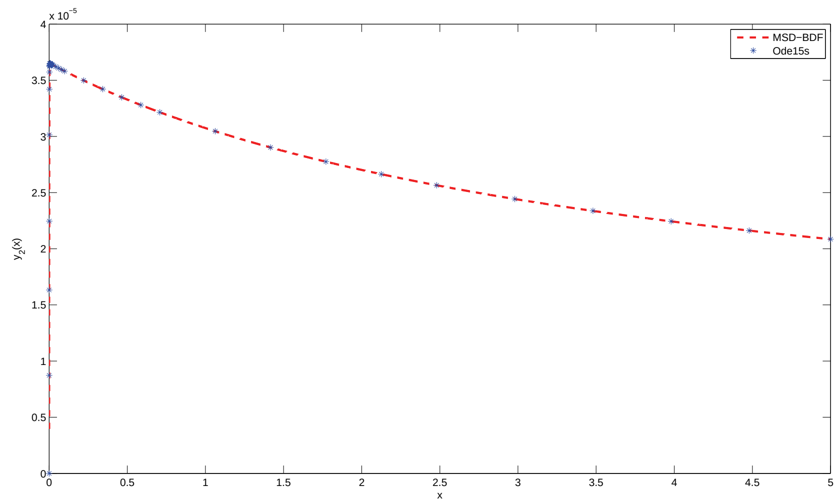

Figure 6: The plot of numerical solutions of $y_2(x)$ component of the nonlinear chemical stiff IVPs in Prob. 2.

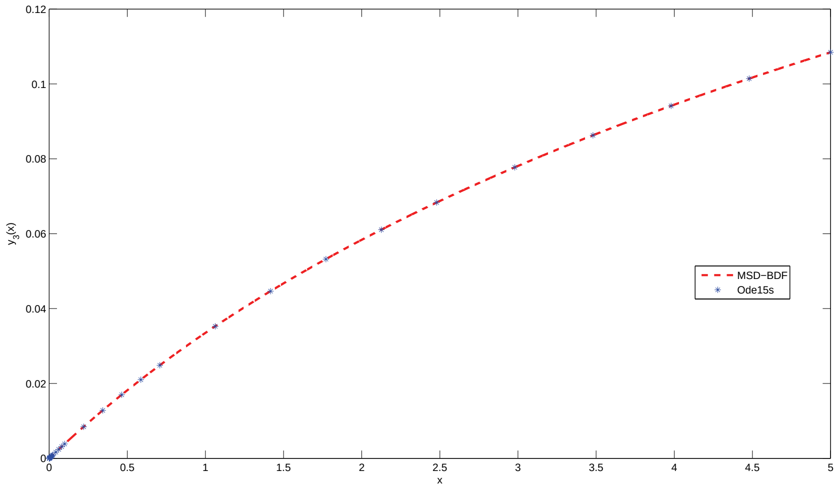

Figure 7: The plot of numerical solutions of $y_3(x)$ component of the nonlinear chemical stiff IVPs in Prob. 2.

6 Concluding remarks

In this paper, we have described an approach to the construction of MSD-BDF (2) of high order and we derived many examples of such formula for step number $k \leq 7$ which is of order $p = k + 1$. The obtained methods are all implicit, they were also found to be A-stable for $k \leq 3$ and stiffly stable for $k = 4(1)7$. The boundary locus in Fig. 1 revealed that the instability of the methods in (2) set in when $k \geq 8$. The numerical solutions in Tables 3 and 4, of the methods in (2) and (3) show that the methods in (2) is compared with the state-of the-art of MATLAB ode15s code in [22], on prob. 1 and prob. 2 respectively.

Acknowledgement The author is grateful to Professor J. C. Butcher, Department Mathematics, University of Auckland, New Zealand for his seminar on the 28th of May, 2010 in University of Benin, Benin City, Nigeria via Skype.

References

[1] Butcher, J. C.: *A modified multistep method for the numerical integration of ordinary differential equations.* J. Assoc. Comput. Mach. **12** (1965), 124–135.

[2] Butcher, J. C.: The Numerical Analysis of Ordinary Differential Equation: Runge Kutta and General Linear Methods. *Wiley*, Chichester, 1987.

[3] Butcher, J. C.: *Some new hybrid methods for IVPs.* In: Cash J.R., Gladwell I. (eds) Computational Ordinary Differential Equations *Clarendon Press*, Oxford, 1992, 29–46.

[4] Butcher, J. C.: *High Order A-stable Numerical Methods for Stiff Problems.* Journal of Scientific Computing **25** (2005), 51–66.

[5] Butcher, J. C.: *Forty-five years of A-stability.*. In: Numerical Analysis and Applied Mathematics: International Conference on Numerical Analysis and Applied Mathematics 2008. AIP Conference Proceedings **1048** (2008).

[6] Butcher, J. C.: Numerical Methods for Ordinary Differential Equations. sec. edi., *Wiley*, Chichester, 2008.

[7] Butcher, J. C.: *General linear methods for ordinary differential equations.* Mathematics and Computers in Simulation **79** (2009), 1834–1845.

[8] Butcher, J. C.: *Trees and numerical methods for ordinary differential equations.* Numerical Algorithms **53** (2010), 153–170.

[9] Butcher, J. C., Hojjati, G.: *Second derivative methods with RK stability.* Numer. Algorithms **40** (2005), 415–429.

[10] Butcher, J. C., Rattenbury, N.: *ARK Methods for Stiff Problems.* Appl. Numer. Math. **53** (2005), 165–181.

[11] Coleman, J. P., Duxbury, S. C.: *Mixed collocation methods for* $y'' = f(x, y)$. Research Report NA-99/01, 1999 *Dept. Math. Sci., University of Durham*, J. Comput. Appl. (2000), 47–75.

[12] Dahlquist, G.: *On stability and error analysis for stiff nonlinear problems. Part 1.* Report No TRITA-NA-7508, *Dept. of Information processing, Computer Science, Royal Inst. of Technology*, Stockholm, 1975.

[13] Enright, W. H.: *Second derivative multistep methods for stiff ODEs.* SIAM J. Num. Anal. **11** (1974), 321–331.

[14] Enright, W. H.: *Continuous numerical methods for ODEs with defect control.* J. Comput. Appl. Math. **125** (2000), 159–170.

[15] Enright, W. H., Hull, T. E., Linberg, B.: *Comparing numerical Methods for Stiff of ODEs systems.* BIT **15** (1975), 1–48.

[16] Fatunla, S. O.: Numerical Methods for Initial Value Problems in ODEs. *Academic Press*, New York, 1978.

[17] Forrington, C. V. D.: *Extensions of the predictor-corrector method for the solution of systems of ODEs.* Comput. J. **4** (1961), 80–84.

[18] Gear, C. W.: *The automatic integration of stiff ODEs.* In: Morrell A.J.H. (ed.) Information processing 68: Proc. IFIP Congress, Edinurgh, 1968 *Nort-Holland*, Amsterdam, 1968, 187–193.

[19] Gear, C. W.: *The automatic integration of ODEs.* Comm. ACM **14** (1971), 176–179.

[20] Gragg, W. B., Stetter, H. J.: *Generalized multistep predictor corrector methods.* J. Assoc. Comput. Mach. **11** (1964), 188–209.

[21] Hairer, E., Wanner, G.: Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems. *Springer-Verlag*, Berlin, 1996.

[22] Higham, J. D., Higham, J. N.: Matlab Guide. *SIAM*, Philadelphia, 2000.

[23] Ikhile, M. N. O., Okuonghae, R. I.: *Stiffly stable continuous extension of second derivative LMM with an off-step point for IVPs in ODEs.* J. Nig. Assoc. Math. Phys. **11** (2007), 175–190.

[24] Kohfeld, J. J., Thompson, G. T.: *Multistep methods with modified predictors and correctors.* J. Assoc. Comput. Mach. **14** (1967), 155–166.

[25] Lambert, J. D.: Numerical Methods for Ordinary Differential Systems. The Initial Value Problems. *Wiley*, Chichester, 1991.

[26] Lambert, J. D.: Computational Methods for Ordinary Differential Systems. The Initial Value Problems. *Wiley*, Chichester, 1973.

[27] Okuonghae, R. I.: *Stiffly Stable Second Derivative Continuous LMM for IVPs in ODEs.* Ph.D. Thesis, *Dept. of Maths. University of Benin*, Benin City. Nigeria, 2008.

[28] Okuonghae, R. I.: *A class of Continuous hybrid LMM for stiff IVPs in ODEs.* Scientific Annals of AI. I. Cuza University of Iasi, (2010), Accepted for publication.

[29] Okuonghae, R. I., Ikhile, M. N. O.: *A continuous formulation of $A(\alpha)$-stable second derivative linear multistep methods for stiff IVPs and ODEs.* J. of Algorithms and Comp. Technology, (2011), Accepted for publication.

[30] Okuonghae, R. I., Ikhile, M. N. O.: *$A(\alpha)$-stable linear multistep methods for stiff IVPs and ODEs.* Acta. Univ. Palacki. Olomuc., Fac. rer. nat., Math. **50** (2011), 73–90.

[31] Selva, M., Arevalo, C., Fuherer, C.: *A Collocation formulation of multistep methods for variable step-size extensions.* Appl. Numer. Math. **42** (2002), 5–16.

[32] Widlund, O.: *A note on unconditionally stable linear multistep methods.* BIT **7** (1967), 65–70.