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High order boundary value linear multistep method for the numerical solution of IVPs in ODEs

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Abstract

In this paper, we introduce High order boundary value linear multistep method (HOBVLMM) for the numerical solution of stiff systems of initial value problems (IVPs). The order, error constant, zero stability and the region of absolute stability for the HOBVLMM are discussed. The proposed scheme posses $0_{k,k-1}$-stability and $(A_{k,k-1})$-stability, achieving a high order of $p = 2k - 1$, where k represents the step number of the LMM. The methods prove to be effective for stiff systems of IVPs in ordinary differential equations (ODEs), as evidenced by our numerical experiments, which shows superior performance compared to some existing methods.

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1. Introduction

Consider the system of IVPs,

$$y' = f(t, y), \quad t \in (t_0, T) \quad y(t_0) = y_0 \in R^m, \tag{1}$$

in ODEs. The continuous IVPs in eq. (1) is often approximated by the classical linear multistep methods (LMMs)

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}, \quad k \geq 1, \quad \alpha_k = 1. \tag{2}$$

Generally, the implementation of LMMs on a system of ODEs as described in eq. (1) involves a step-by-step procedure detailed in [1, 2], with backward differentiation formulas (BDFs) being an example of such a class of LMMs [3, 4].

$$\sum_{j=0}^{k} a_j y_{n+j} = h f_{n+k}; \quad k = 1, \cdots, 6, \quad p = k, \tag{3}$$

where y_n is the discrete approximation of the theoretical solution $y(t_n)$ at the point $t_n = t_0 + nh$, $f_n = f(t_n, y_n)$ is the function evaluated at t_n, and h is the step size of the LMMs.

The method in eq. (3) is an essential scheme for approximating ODEs in eq. (1). As an initial value method, the methods in eq. (3) require the past solutions $y_{n+1}, y_{n+2}, \ldots, y_{n+k-1}$ at the initial step ($n = 0$) to compute y_k, with y_0 given by the continuous problem in eq. (1). However, BDFs in eq. (3), like other LMMs in eq. (2), are subject to the Dahlquist barrier [5]. Specifically, these schemes are A-stable for $k \leq 2$, $A(\alpha)$-stable for $k = 3, 4, 5, 6$, and unstable for $k \geq 7$.

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Consequently, the extended backward differentiation formulas (EBDF)

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=k}^{k+1} \beta_j f_{n+j}; \quad k \geq 1, \quad p = k+1, \tag{4}$$

which uses the future solution y_{n+k+1} at the future point t_{n+k+1}, have been introduced by Cash [6] and used in composition with BDFs in eq. (3). Cash's methods are A-stable for $k \leq 3$ and stiffly stable for $k \leq 8$.

Cash [7] similarly improved these methods by introducing second derivative BDFs for the approximation of stiff systems in eq. (1). Stiff systems in eq. (1) are ODEs with Jacobians having some widely dispersed eigenvalues on the complex plane $\mathbb{C}^-$.

The authors in Refs. [8–12] have considered different classes of methods that also employ future points as in eq. (4) and higher derivatives to circumvent the Dahlquist order-stability limitation of the method in eq. (2). The A-stability properties for the LMM in eq. (2) was also improved by introducing off-grid point (see Refs. [13–16]). However, a different approach was considered in Refs. [17–21] , where the continuous IVPs in eq. (1) are addressed using discrete boundary value problems (BVPs). The schemes derived in this manner are known as boundary value methods (BVMs). BVMs are free from the Dahlquist [22] order and stability barrier, unlike the LMMs in eq. (2). An example of such a scheme is:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h f_{n+v}; \quad k \geq 1, \quad N \geq k, \tag{5}$$

$$y_0, y_1, y_2, \cdots, y_{v-1}, \quad y_{N-k+v+1}, \cdots, y_N \quad \text{(provided)},$$

which transform BDFs in eq. (3) to a BVM with v defined as (see [19])

$$v = \begin{cases} \frac{k+2}{2}; & \text{even} \\ \frac{k+1}{2}; & \text{odd.} \end{cases} \tag{6}$$

The BVM in eq. (5) is $0_{v,k-v}$-stable and $A_{v,k-v}$-stable, thus it is employed with $(v, k-v)$-boundary conditions. Generally, BVMs are effective numerical methods for solving IVPs and BVPs, as detailed in Refs. [23–32]. For further information, refer to the monographs by Brugnano and Trigiante [19]. The application of BVMs and Block BVMs has proven effective in approximating solutions for delay differential equations (DDEs), differential algebraic equations (DAEs) and Volterra integro-differential equations [33–38]. Additionally, BVMs have been applied to neutral equations, neutral multi-DDEs and fractional differential equations in Refs. [39–42]. The documentation of multi-block boundary value methods that generate multi-block of solutions per output and its root distribution procedure are in Ogunfeyitimi and Iknile [43, 44]. This article is organized as follows: in Section 2, we will discuss some properties of BVMs. In Section 3, we describe the derivation and analysis of the methods. Section 4 details the implementation procedures for the methods. Numerical experiments are presented in Section 5. Lastly, concluding remarks are provided in Section 6.

2. The boundary-value methods (BVMs)

The application of the discretization method in eq. (2) as a BVM assumes that the continuous IVPs in eq. (1) can be reduced to a BVPs. Thus we can impose additional initial and final conditions on the solution values of the ODEs in eq. (1) at the boundaries of interest in the method. Thus, given a k-step method in eq. (2) for the approximation of the solution of eq. (1) [19], then for the BVM:

$$\sum_{j=-k_1}^{k_2} \alpha_j y_{n+j} = h \sum_{j=-k_1}^{k_2} \beta_j f_{n+j}, \tag{7}$$

$$k_1, k_2 \in N, \quad n = k_1, \cdots, N-k_2,$$

is the main formula ($k_1 + k_2 = k$), while the initial and final conditions on implementation on eq. (1) are determined by providing the solution inputs,

$$y_0, y_1, y_2, \cdots, y_{k_1-1}; \quad y_{N-k_2+1}, \cdots, y_N, \tag{8}$$

respectively. These values are obtained by solving simultaneously k_1 number of linear mutistep formulas(LMFs) of similar form to eq. (7) at initial points in the integration interval and k_2 number of LMFs at final points of the integration interval along with those induced by the main method. By this the method in eq. (7) can be used with $(k_1, k_2)-$boundary conditions (see [19], definition 4.7.1, page 101). The k_1 and k_2 is associated with the root distribution type $(k_1, 0, k_2)$ of the method in eq. (7). In fact, the initial solution values in eq. (8) can be obtained from

$$\sum_{j=0}^{k} \alpha_j^{(i)} y_j = h \sum_{j=0}^{k} \beta_j^{(i)} f_j; \quad i = 1, \cdots, k_1 - 1, \tag{9}$$

and the final ones

$$\sum_{j=0}^{k} \alpha_{k-j}^{(i)} y_{N-j} = h \sum_{j=0}^{k_2} \beta_{k-j}^{(i)} f_{N-j}, \quad i = N-k_2+1, \cdots, N. \tag{10}$$

For proper understanding of BVMs, the subsequent definitions are required. Let the two characteristics equation associated with eq. (2) be:

$$\rho(r) = \sum_{j=0}^{k} \alpha_j r^j; \quad \sigma(r) = \sum_{j=0}^{k} \beta_j r^j. \tag{11}$$

For any complex $z = \lambda h$, we have

$$\prod(r, z) = \sum_{j=0}^{k} \alpha_j r^j - z \sum_{j=0}^{k} \beta_j r^j; \qquad z = \lambda h, \tag{12}$$

as the stability equation when eq. (2) is applied to the usual scalar test problem equation $y' = \lambda y$, $Re(\lambda) < 0$. Thus from [18, 19], we have:

Definition 2.1. A polynomial $\rho(r)$ of degree $k = k_1 + k_2$ is an $S_{k_1,k_2}-$polynomial, if its roots $\{r_j\}_{j=1}^{k}$ satisfy the condition $|r_1| \leq |r_2| \leq \cdots \leq |r_{k_1}| < 1 < |r_{k_1+1}| \leq \cdots \leq |r_k|$.

Definition 2.2. A polynomial $\rho(r)$ of degree $k = k_1 + k_2$ is an N_{k_1,k_2}−polynomial, if its roots $\{r_j\}_{j=1}^{k}$ satisfy the condition $|r_1| \le |r_2| \le \cdots \le |r_{k_1}| \le 1 < |r_{k_1+1}| \le \cdots \le |r_k|; \quad |r_{k_1}| = 1$.

If $k_1 = k$, $k_2 = 0$, definition 2.2 becomes a Von Neumann polynomial and definition 2.1 is transformed into a Schur polynomial, similarly to the LMFs in eq. (2) in which are IVMs governed by the Dahlquist [5] stability criteria.

Definition 2.3. (cf. [19]) The scheme in eq. (7) with (k_1, k_2) −boundary condition where $k = k_1 + k_2$ is:

(a) O_{k_1,k_2}−stable if the associated polynomial $\rho(r)$ in (11) satisfy definition 2.2.

(b) (k_1, k_2) −absolutely stable, if $\prod(r, z)$ in (12) satisfy definition 2.1.

(c) The region $D_{k_1,k_2} = \{z \in \mathbb{C} : \prod(r, z)$ satisfy definition 2.1$\}$ is said to be the region of (k_1, k_2) −absolute stability.

(d) A_{k_1,k_2}−stable if $\mathbb{C}^- \subseteq D_{k_1,k_2}$.

3. Derivation of the methods

Adopting the approach of Brugnano and Trigiante [19, 25], we write the generalized form of the extended BDF in eq. (3) (see, [4, 6]) in the form

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=k}^{2k-1} \beta_j f_{n+j}; \quad k \ge 1, \quad \alpha_k = 1, \tag{13}$$

as the main formula which employs in the sense of LMMs in eq. (2) with the future solution values $\{y_{n+j}\}_{j=k+1}^{2k-1}$ compared to eq. (2) and eq. (4), while the initial and final LMFs associated with eq. (13) are determined by fixing the input values,

$$y_0, y_1, y_2, \cdots, y_{k-1}; \quad y_{N-k+2}, \cdots, y_N, \tag{14}$$

at the points t_0, t_1,$\cdots$, t_{k-1} and t_{N-k+2}, t_{N-k+3},$\cdots$,t_N respectively. Thus for $k = 1$ in eq. (13) is the conventional BDF (implicit Euler method) of order $p = 1$. The $2k$ parameters $\{\alpha_j\}_{j=0}^{k-1}$ and $\{\beta_{k+j}\}_{j=0}^{k-1}$ are determine such that the methods in eq. (13) is of maximum order $p = 2k - 1$.

Remark 1. The first characteristics equations $\rho(r)$ for the schemes eq. (13) is of degree $2k - 1$ with $k - 1$ number of zeros at ∞, that is,

$$\alpha_{2k-1} = \alpha_{2k-2} = \cdots = \alpha_{k+1} = 0; \qquad k > 1.$$

The methods in eq. (13) are $0_{k,k-1}$-stable, $A_{k,k-1}$−stable and thus used along with $(k, k - 1)$ −boundary conditions. The high order boundary value linear multistep method (HOBVLMM) in eq. (13) as $(k - 1)$ future points at $\{t_{n+j}\}_{j=k+1}^{2k-1}$ and the corresponding future solutions are $\{y_{n+j}\}_{j=k+1}^{2k-1}$ (see Ref. [4]). The HOBVLMM in eq. (13) has $2k - 1$ order arising from the fact that

$$\sum_{j=0}^{k} \alpha_j y(t + jh) - h \sum_{j=k}^{2k-1} \beta_j y'(t + jh) = C_{2k} h^{2k} y^{(2k)}(t) + O\left(h^{2k+1}\right). \tag{15}$$

The coefficients of the methods in eq. (13) are presented in Tables 1 and 2.

3.1. The stability procedure for HOBVLMM

As described in Ref. [2], the linear difference operator $\mathbf{L}[y(t), h]$ associating to LMFs in eq. (13) is:

$$\mathcal{L}[y(t); h] = \sum_{j=0}^{k} \alpha_j y(t + jh) - h \sum_{j=k}^{2k-1} \beta_j y'(t + jh). \tag{16}$$

As observed from eq. (15), the function $y(t)$ is sufficiently differentiable. The eq. (16) provides the local truncation error (*lte*) of the LMFs in eq. (13), with $y(t)$ assumed to be the theoretical solution of eq. (1). Let $y(t)$ be atleast $(p + 1)$ times continuously differentiable, then we have,

$$\begin{aligned} \mathcal{L}(y(t); h) = \; & C_0 y(t) + C_1 h y'(t) + \cdots + C_p h^p y^{(p)}(t) \\ & + C_{p+1} h^{p+1} y^{(p+1)}(t) + \cdots, \end{aligned} \tag{17}$$

by expanding eq. (16) through Taylor series approach. Here

$$\left.\begin{aligned} & C_0 = \textstyle\sum_{j=0}^{k} \alpha_j; \quad C_1 = \sum_{j=0}^{k} j\alpha_j - \sum_{j=k}^{2k-1} \beta_j; \\ & C_2 = \textstyle\sum_{j=0}^{k} \frac{j^2}{2!}\alpha_j - \sum_{j=k}^{2k-1} j\beta_j; \cdots \\ & C_p = \textstyle\sum_{j=0}^{k} \frac{j^p}{p!}\alpha_j - \sum_{j=k}^{2k-1} \frac{j^{p-1}}{(p-1)!}\beta_j \quad p \ge 1, \quad k \ge 1. \end{aligned}\right\} \tag{18}$$

The order of the LMF in eq. (13) is defined in what now follows.

Definition 3.1. The HOBVLMM in eq. (13) are of order p, if

$$C_0 = C_1 = C_2 = \cdots C_p = 0; \quad p \ge 1,$$

with the error constant $C_{p+1} \ne 0$ and

$$lte = C_{p+1} h^{p+1} y^{(p+1)}(t) + O\left(h^{p+2}\right). \tag{19}$$

As the principal local trruncation errorr (lte).

By comparing with the generalized backward differentiation formulas (GBDF) [19] and the extended backward differentiation formulas (*EBDF*) [6]. It has been determined that the method in eq. (7) achieves a higher order of $2k - 1$, and results in smaller error constants for the equivalent step number k as shown in Figure 1.

Now, following eq. (11),

$$\begin{aligned} & \rho(r) = \textstyle\sum_{j=0}^{k} \alpha_j r^j, \\ & \sigma(r) = r^k \left(\beta_k + \beta_{k+1} r + \cdots + \beta_{2k-1} r^{k-1}\right), \end{aligned} \tag{20}$$

are the two characteristics equation corresponding with eq. (13) respectively. The stability polynomial in eq. (12) for eq. (13) is given as

$$\begin{aligned} & \prod(r, z) = \textstyle\sum_{j=0}^{k} \alpha_j r^j - z \sum_{j=k}^{2k-1} \beta_j r^j; \\ & z = h\lambda; \quad z = e^{j\theta}; \quad \theta \in [0, 2\pi]. \end{aligned} \tag{21}$$

This is used to obtain the boundary of the stability region determined through its locus as in Figure 2 and 3. The stability of the polynomial under A_{k_1,k_2}−stable ensures that the root distribution remains invariant as z changes within $\mathbb{C}^-$. The boundary locus is

$$\Gamma = \left\{ z \in \mathbb{C} : z = \frac{\rho\left(e^{i\theta}\right)}{\sigma\left(e^{i\theta}\right)}, \quad 0 \le \theta \le 2\pi, \quad Re(z) < 0 \right\}, \tag{22}$$

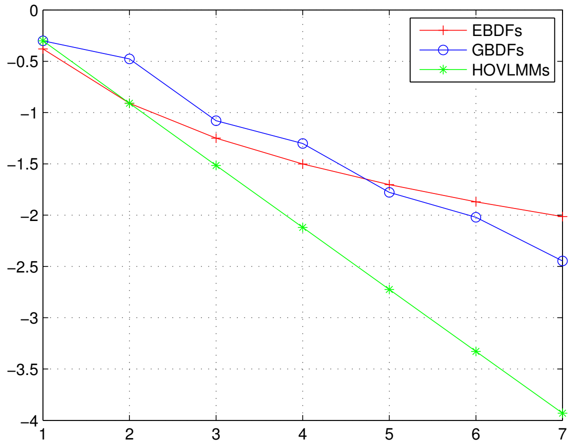

Figure 1: The plot of error constants versus step number of the HOBVLMM (13), generalized backward differentiation formulas (GBDF) [19] and the extended backward differentiation formulas ($EBDF$) [6].

and belongs to $\mathbb{C}\backslash\mathbb{C}^-$ for methods with unbounded stability region, see Figure 2 and 3. The stability region of the BVMs in eq. (13) is the outermost simple closed curves denoted by Γ. Here $k_1 = k$, $k_2 = k - 1$ in eq. (13). The second characteristics stability polynomial $\sigma(r)$ in eq. (20) determines the stability of the LMF in eq. (13) as $z \to \infty$.

The following examples confirm the definition 2.1 and 2.2 for the methods in eq. (13).

Example 1.
The stability polynomial of third order method in eq. (13) for $k = 2$ (see, (33)) is:

$$\prod(r,z) = \frac{5}{23} - \frac{28r}{23} + r^2 - \frac{22r^2z}{23} + \frac{4r^3z}{23}. \tag{23}$$

By setting $z = 0$ in eq. (23), the root distribution is obtained by finding the values of r, which gives one root inside the unit circle, one root on the boundary and one root at infinity,

$$r_1 = 0.217391, \qquad r_2 = 1 \quad \text{and} \quad r_3 \quad \text{at} \quad \infty. \tag{24}$$

Thus the HOBVLMM in eq. (13) for $k = 2$ is a $N_{2,1}$-polynomial with root distribution type $(1, 1, 1)$, see remark 1.
Similarly, choosing the value of $z = -20 + i$ (from exterior of closed curve) for eq. (23) gives rise to:

$$\begin{aligned} &r_1 = 0.0273389 + 0.101521i, r_3 = 5.72772 + 0.0115012i. \\ &r_2 = 0.0317202 - 0.0986835i. \end{aligned} \quad .(25)$$

This indicates that the method in eq. (13) for $k = 2$ is $S_{2,1}$-polynomial and is of the type $(2, 0, 1)$.

Example 2.
The stability polynomial of fifth order method in eq. (13) for $k = 3$ is,

$$\prod(r,z) = \begin{aligned} &-\tfrac{413}{8018} + \tfrac{1467r}{4009} - \tfrac{10539r^2}{8018} + r^3 - \tfrac{7503r^3z}{8018} \\ &+\tfrac{963r^4z}{4009} - \tfrac{333r^5z}{8018}. \end{aligned} \tag{26}$$

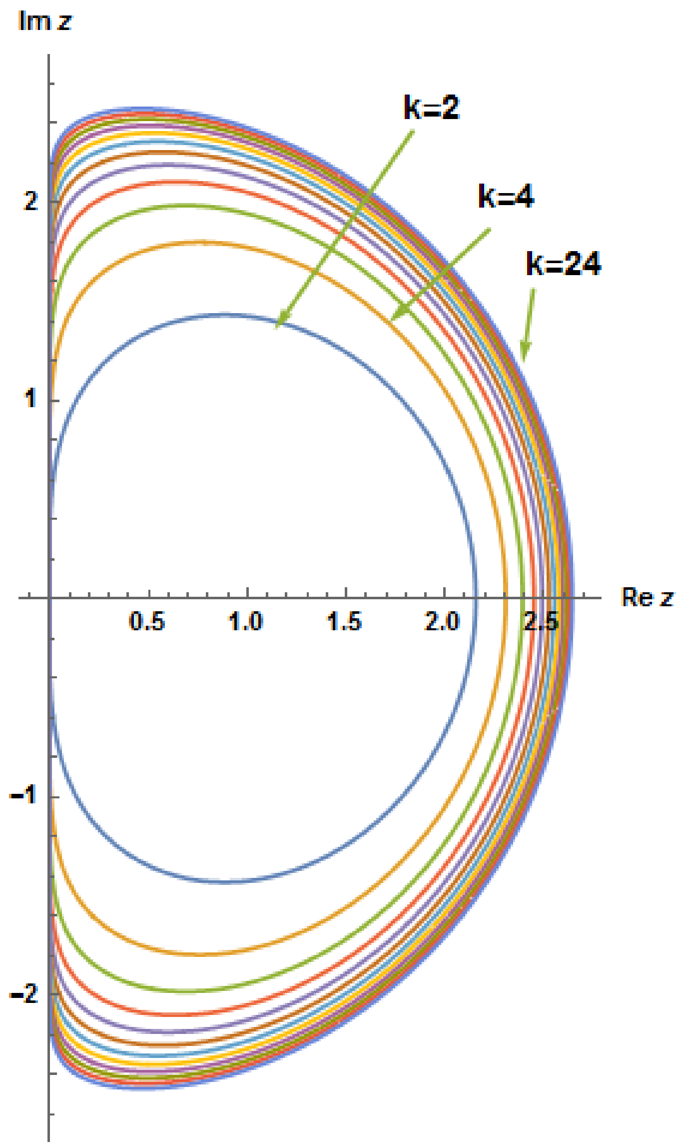

Figure 2: Boundary locus of the stability regions of the HOBVLMM in eq. (13) of order $p = 2k - 1$, $k = 2(2)24$.

By setting $z = 0$ in eq. (26), the root distribution contain two root inside the unit circle, one root on the boundary and two root at infinity,

$$\begin{aligned} &r_1 = 0.157209 - 0.16369i, \\ &r_2 = 0.157209 + 0.16369i, \\ &r_3 = 1 \quad \text{and} \quad r_4, r_5 \quad \text{at} \quad \infty. \end{aligned} \tag{27}$$

The HOBVLMM in eq. (13) for $k = 3$ is a $N_{3,2}$-polynomial with root distribution type $(2, 1, 2)$. While, the value of $z = -20 + i$ (from exterior of closed curve) for in eq. (26) gives rise to,

$$\begin{aligned} &r_1 = -0.0272322 + 0.152592i, r_4 = 2.85388 + 3.8936i \\ &r_2 = -0.021754 - 0.151166i, r_5 = 2.86688 - 3.89664i \\ &r_3 = 0.112018 + 0.00162275i. \end{aligned} \tag{28}$$

Thus the scheme in eq. (13) for $k = 3$ is $S_{3,2}$-polynomial and is of the type $(3, 0, 2)$.

Table 1: Coefficients $\left\{\alpha_j, \beta_j\right\}$ of HOBVLMM in eq. (13).

k	α_0	α_1	α_2	α_3	α_4	α_5	β_k
1	$-\frac{1}{2}$	$\frac{1}{2}$	0	0	0	0	$\frac{1}{2}$
2	$\frac{5}{46}$	$-\frac{28}{46}$	$\frac{1}{2}$	0	0	0	$\frac{22}{46}$
3	$-\frac{413}{16036}$	$\frac{1467}{8018}$	$-\frac{10539}{16036}$	$\frac{1}{2}$	0	0	$\frac{7503}{16036}$
4	$\frac{547411}{87552802}$	$-\frac{4892864}{87552802}$	$\frac{20541276}{87552802}$	$-\frac{59972224}{87552802}$	$\frac{1}{2}$	0	$\frac{40423284}{43776401}$
5	$-\frac{23200008502}{7562497020627}$	$\frac{251828397925}{7562497020627}$	$-\frac{425286340600}{2520832340209}$	$\frac{4118878208200}{7562497020627}$	$-\frac{10634144596450}{7562497020627}$	1	$\frac{2306800631670}{2520832340209}$

Table 2: Coefficients $\left\{\alpha_j, \beta_j\right\}$ of HOBVLMM in eq. (13) (continuation).

k	β_{k+1}	β_{k+2}	β_{k+3}	β_{k+4}	p	C_{p+1}
1	0	0	0	0	1	$-\frac{1}{2}$
2	$-\frac{4}{23}$	0	0	0	3	$\frac{17}{138}$
3	$-\frac{963}{8018}$	$\frac{33}{16036}$	0	0	5	$-\frac{979}{32072}$
4	$-\frac{11992752}{43776401}$	$\frac{3393672}{43776401}$	$-\frac{445584}{43776401}$	0	7	$\frac{40423284}{43776401}$
5	$-\frac{741030532400}{2520832340209}$	$\frac{266004453800}{2520832340209}$	$-\frac{60566107800}{2520832340209}$	$\frac{6342120150}{2520832340209}$	9	$-\frac{599639466667}{31762487866334}$

4. Implementation procedure of the methods

In this section, we give an illustration for the implementation of the schemes in eq. (13) as BVM inline with Brugnano and Trigiante [19], Ogunfeyitimi and Ikhile [30]. The new scheme in eq. (13) is completely used with $(k, k-1)$-boundary conditions or, coupled with an extra 2k-1 additional equations since the IVPs in eq. (1) gives the initial value y_0. Thus,the $k-1$ additional initial solution $y_1, \cdots, y_{k-1}$ for eq. (13) can be obtained from the LMFs of the form:

$$\sum_{j=0}^{2k-1} \alpha_j^{(i)} y_j = h\beta_i^{(i)} f_i; \quad i = 1, \cdots, k-1, \tag{29}$$

and the $k-1$ final discrete solution $y_{N-k+2}, \cdots, y_N$ are similarly obtained from the LMFs,

$$\sum_{j=0}^{2k-1} \alpha_j^{(i)} y_{N-2k+1+j} = h\beta_i^{(i)} f_{N-2k+1+i}; \quad i = k+1, \cdots, 2k-1. \tag{30}$$

In particular, the composite scheme of eq. (13), eq. (29) and eq. (30) is a BVM of uniform order $p = 2k-1$ and is conveniently written as a one block method of the form

$$AY_{n+1} + A_0 Y_n = h(BF_{n+1} + B_0 F_n), \tag{31}$$

with output block of solution values, where:

$$\begin{aligned} Y_{n+1} &= (y_{n+1}, y_{n+2}, \cdots, y_{n+k_1}, y_{n+k_1+1}, \cdots, y_{n+N-k_2}, y_{n+N-k_2+1}, \cdots, y_{n+N})^T \\ F_{n+1} &= (f_{n+1}, f_{n+2}, \cdots, f_{n+k_1}, f_{n+k_1+1}, \cdots, f_{n+N-k_2}, f_{n+N-k_2+1}, \cdots, f_{n+N})^T, \end{aligned} \tag{32}$$

with the matrix coefficients $A_0 = [\mathbf{0}_{N\times N-1} \mid a_0] \in R^{N\times N}$ and $B_0 = [\mathbf{0}_{N\times N-1} \mid b_0] \in R^{N\times N}$. The matrix $[a_0 \mid A] \in R^{(N)\times(N+1)}$ is

$$[a_0 \mid A] = \left(\begin{array}{c|cccccc} \alpha_0^{(1)} & \alpha_1^{(1)} & \cdots & \alpha_k^{(1)} & & & \\ \vdots & \vdots & & \vdots & & & \\ \alpha_0^{(k_1-1)} & \alpha_1^{(k_1-1)} & \cdots & \alpha_k^{(k_1-1)} & & & \\ \alpha_0 & \alpha_1 & \cdots & \alpha_k & & & \\ 0 & \alpha_0 & \alpha_1 & \cdots & \alpha_k & & \\ & & \ddots & \ddots & \ddots & \ddots & \\ & & & \alpha_0 & \alpha_1 & \cdots & \alpha_k \\ & & & \alpha_0^{(N-k_2+1)} & \alpha_1^{(N-k_2+1)} & \cdots & \alpha_k^{(N-k_2+1)} \\ & & & \vdots & \vdots & \cdots & \vdots \\ & & & \alpha_0^{(N)} & \alpha_1^{(N)} & \cdots & \alpha_k^{(N)} \end{array}\right),$$

and the matrix $[b_0 \mid B]$ is of equivalent nature with β_j in place of α_j and $\beta'_j s$ in place of $\alpha'_j s$.

Definition 4.1. The composite scheme in eq. (31) is pre-consistent if $\| A^{-1}\alpha \|_\infty = 1$ holds.

Thus, the implementation of the BVMs as a one block form in eq. (31) is achieved by using a modified Newton-Raphson method for non linear problem while for linear problem, one require Guassian elimination using partial pivoting. These are employed in the numerical experiments in section 5. For example, considering the third order HOBVLMM (denoted by HOBVLMM2) from eq. (13):

$$\frac{5y_n}{23} - \frac{28y_{n+1}}{23} + y_{n+2} = h\left(\frac{22f_{n+2}}{23} - \frac{4f_{n+3}}{23}\right), \quad n = 0, \cdots, N-3, \tag{33}$$

which is $A_{2,1}-$stable and thus applied on eq. (1) with the one initial formula

$$-\frac{y_0}{3} - \frac{y_1}{2} + y_2 - \frac{y_3}{6} = hf_1, \tag{34}$$

and one final formula

$$-\frac{y_{N-3}}{33} + \frac{3y_{N-2}}{22} - \frac{3y_{N-1}}{11} + \frac{y_N}{6} = \frac{1}{11}hf_N. \tag{35}$$

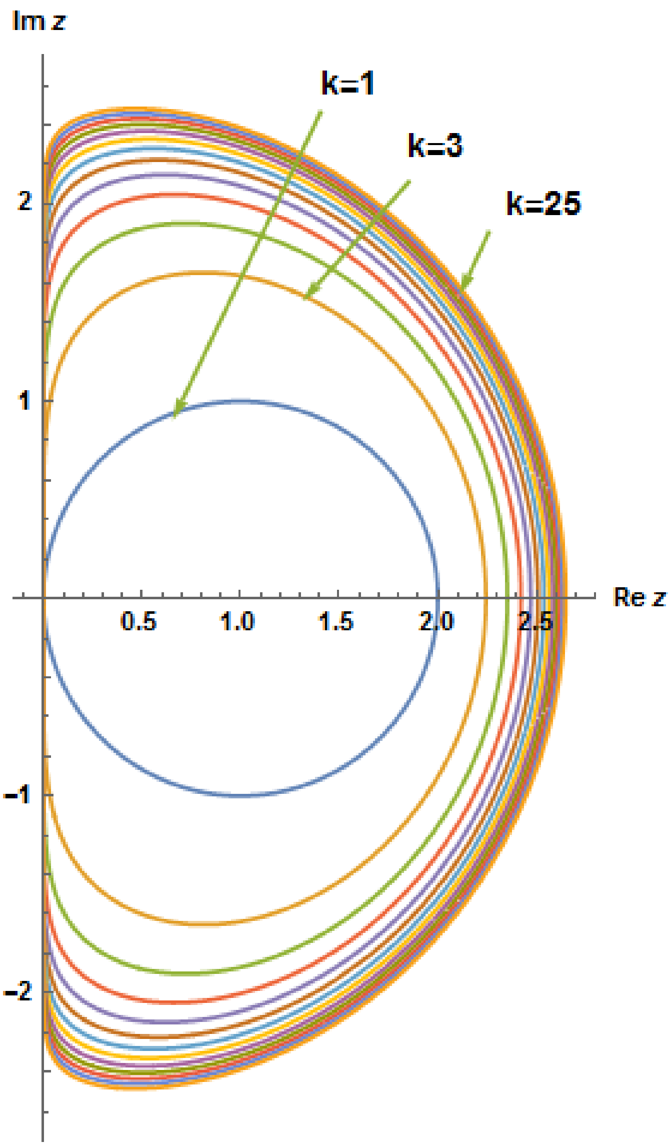

Figure 3: Boundary locus of the stability regions of the HOBVLMM in eq. (13) of order $p = 2k - 1$, $k = 1(2)25$.

The fifth order HOBVLMM (HOBVLMM3) from eq. (13):

$$-\frac{413}{16036}y_n + \frac{1467}{8018}y_{n+1} - \frac{10539}{16036}y_{n+2} + \frac{1}{2}y_{n+3} = \frac{h}{16036}\Big(7503f_{n+3} -1926f_{n+4} + 333f_{n+5}\Big), \quad n = 0, \cdots, N-5, \tag{36}$$

is $A_{3,2}-$stable and thus implemented with the following two initial formulas:

$$\begin{aligned} -\frac{y_0}{15} - \frac{13y_1}{36} + \frac{2y_2}{3} - \frac{y_3}{3} + \frac{y_4}{9} - \frac{y_5}{60} &= h\frac{f_1}{3} \\ \frac{y_0}{40} - \frac{y_1}{4} - \frac{y_2}{6} + \frac{y_3}{2} - \frac{y_4}{8} + \frac{y_5}{60} &= h\frac{f_2}{2}, \end{aligned} \tag{37}$$

and two final formulas

$$\begin{aligned} \frac{y_{N-5}}{60} - \frac{y_{N-4}}{9} + \frac{y_{N-3}}{3} - \frac{2y_{N-2}}{3} + \frac{13y_{N-1}}{36} + \frac{y_N}{15} &= \frac{hf_{N-1}}{3} \\ -\frac{y_{N-5}}{30} + \frac{5y_{N-4}}{24} - \frac{10y_{N-3}18}{+}\frac{5y_{N-2}}{6} - \frac{5y_{N-1}}{6} + \frac{137y_N}{360} &= \frac{hf_N}{6}. \end{aligned} \tag{38}$$

The seventh order HOBVLMM (HOBVLMM4) from eq. (13):

$$\begin{aligned} &\frac{547411y_n}{43776401} - \frac{4892864y_{n+1}}{43776401} + \frac{20541276y_{n+2}}{43776401} - \frac{59972224y_{n+3}}{43776401} + y_{n+4} \\ &= h\Big(\frac{40423284f_{n+4}}{43776401} + \frac{3393672f_{n+6}}{43776401} - \frac{11992752f_{n+5}}{43776401} - \frac{445584f_{n+7}}{43776401}\Big), \\ &\quad n = 0, \cdots, N-7, \end{aligned} \tag{39}$$

is $A_{4,3}-$stable and thus implemented with the following three initial formulas:

$$\begin{aligned} -\frac{y_n}{7} - \frac{29y_{n+1}}{20} + 3y_{n+2} - \frac{5y_{n+3}}{2} + \frac{5y_{n+4}}{3} - \frac{3y_{n+5}}{4} + \frac{y_{n+6}}{5} - \frac{y_{n+7}}{42} &= hf_{n+1} \\ \frac{y_n}{42} - \frac{y_{n+1}}{3} - \frac{47y_{n+2}}{60} + \frac{5y_{n+3}}{3} - \frac{5y_{n+4}}{6} + \frac{y_{n+5}}{3} - \frac{y_{n+6}}{12} + \frac{y_{n+7}}{105} &= hf_{n+2} \\ -\frac{y_n}{105} + \frac{y_{n+1}}{10} - \frac{3y_{n+2}}{5} - \frac{y_{n+3}}{4} + y_{n+4} - \frac{3y_{n+5}}{10} + \frac{y_{n+6}}{15} - \frac{y_{n+7}}{140} &= hf_{n+3}, \end{aligned}$$

and three final formulas

$$\begin{aligned} &-\frac{y_{N-7}}{105} + \frac{y_{N-6}}{12} - \frac{y_{N-5}}{3} + \frac{5y_{N-4}}{6} - \frac{5y_{N-3}}{3} + \frac{47y_{N-2}}{60} + \frac{y_{N-1}}{3} - \frac{y_N}{42} = hf_{N-2} \\ &\frac{y_{N-7}}{42} - \frac{y_{N-6}}{5} + \frac{3y_{N-5}}{4} - \frac{5y_{N-4}}{3} + \frac{5y_{N-3}}{2} - 3y_{N-2} + \frac{29y_{N-1}}{20} + \frac{y_N}{7} = hf_{N-1} \\ &-\frac{y_{N-7}}{7} + \frac{7y_{N-6}}{6} - \frac{21y_{N-5}}{5} + \frac{35y_{N-4}}{4} - \frac{35y_{N-3}}{3} + \frac{21y_{N-2}}{2} - 7y_{N-1} \\ &+\frac{363y_N}{140} = hf_N. \end{aligned}$$

5. Bound of global truncation error of the composite methods

The following condition holds for the global truncation error of the composite methods in eq. (31), since the main methods and the additional methods have the same order.

Lemma 5.1. Suppose that the $\{\epsilon_i, i = 0, 1, \cdots, n\}$ be a set of real numbers. If there exist finite constants W and U such that

$$|\epsilon_{i+i}| \leq aW|\epsilon_i| + U, \quad i = 0, 1, \cdots, n-1; \quad a \geq 1, \tag{40}$$

then

$$|\epsilon_i| \leq \frac{(aW)^i - 1}{aW - 1}U + (aW)^i|\epsilon_0|, \quad W \neq \frac{1}{a}, \quad a \geq 1. \tag{41}$$

Proof. For $i = 0$,eq. (40) is equivalently as $|\epsilon_0| \leq |\epsilon_0|$. Suppose eq. (41) holds for $i \leq k$ so that

$$|\epsilon_k| \leq \frac{(aW)^k - 1}{aW - 1}U + (aW)^k|\epsilon_0|, \tag{42}$$

then for $i = k$, eq. (40) gives:

$$|\epsilon_{k+1}| \leq aW|\epsilon_k| + U, \tag{43}$$

inclusion of eq. (42) into eq. (43) gives:

$$|\epsilon_{k+1}| \leq \frac{(aW)^{k+1} - 1}{aW - 1}U + (aW)^{k+1}|\epsilon_0|, \tag{44}$$

where eq. (41) holds for all $i \geq 0$. □

Theorem 5.1. Assume the effect of round-off error is not significant and the composite methods has atleast order one, then the composite methods in eq. (31) is convergent with global error order $O(h^{2k-1})$.

Proof. Since the composite methods in eq. (31) is employed to solve problem in eq. (1) by utilizing the following initial solution inputs $y_0, y_1, \cdots, y_{k_1}$ and final solution inputs $y_{N-k_1+1}, \cdots, y_N$, where

$$Y_{n+1} = (y_{n+1}, \cdots, y_{n+k_1-1}, y_{n+k}, \cdots, y_{n+N-k_2}, y_{n+N-k_2+1}, \cdots, y_{n+N})^T, \quad (45)$$

$$F_{n+1} = (f_{n+1}, \cdots, f_{n+k_1-1}, f_{n+k}, \cdots, f_{n+N-k_2}, f_{n+N-k_2+1}, \cdots, f_{n+N})^T, \quad (46)$$

is the block solution and function values. According to Lambert (1976), l.t.e (denoted by τ_{n+1}) for the composite methods in eq. (31) is given as:

$$AY_{n+1} + A_0 Y_n = h(BF_{n+1} + B_0 F_n) + \tau_{n+1}, \quad (47)$$

with

$$\tau_{n+1} = C_{2k} h^{2k} Y_{n+1}^{2k}(t_n + ih), \quad 0 < i < 1. \quad (48)$$

Let Ch^{2k} be an upper bound for the l.t.e for the composite methods applied to the scalar test equation $y' = \lambda y$ in $t_0 \le t \le T$, that is

$$\max_{t_0 \le t \le T} \| \tau_{n+1} \| = Ch^{2k}, \quad (49)$$

then eq. (47) can be rewritten as:

$$AY_{n+1} + A_0 Y_n = h\lambda(BY_{n+1} + B_0 Y_n) + \tau_{n+1}, \quad (50)$$

substituting eq. (31) into eq. (50) gives to global truncation error (denoted by ϵ_{n+1})

$$A\epsilon_{n+1} = -A_0 \epsilon_n + h\lambda(B\epsilon_{n+1} + B_0 \epsilon_n) + \tau_{n+1}. \quad (51)$$

Remark 2. $\epsilon_{n+1} = Y_{n+1}(t_n) - Y_{n+1}$ is the differences between the theoretical solution and numerical solution.

Then, it follows that

$$\epsilon_{n+1} = (A - B\lambda h)^{-1} \left[(B_0 \lambda h - A_0) \epsilon_n + \tau_{n+1} \right]. \quad (52)$$

By applying the principle of triangle inequalities gives rise to:

$$\| \epsilon_{n+1} \|_\infty = Q^{-1} \left((B_0 \lambda h - A_0) \| \epsilon_n \|_\infty + \| \tau_{n+1} \|_\infty \right), \quad (53)$$

with $Q = (A - B\lambda h)$. Considering Lemme (5.1) gives:

$$\| \epsilon_n \|_\infty \le Q^{-1} \left(\frac{(aB_0\lambda h - aA_0)^n - I}{aB_0\lambda h - aA_0 - I} Ch^{2k} + (aB_0 \lambda h - aA_0)^n \| \epsilon_0 \|_\infty \right)$$

$$\le Q^{-1} \left(\frac{(aB_0\lambda h - aA_0)^n - I}{aB_0\lambda h - aA_0 - I} Ch^{2k-1} + (aB_0 \lambda h - aA_0)^n \| \epsilon_0 \|_\infty \right). \quad (54)$$

Taking $z = \lambda h$, we have

$$\le Q^{-1} \left(\frac{(aB_0 z - aA_0)^n - I}{aB_0 z - aA_0 - I} Ch^{2k-1} + (aB_0 z - aA_0)^n \| \epsilon_0 \|_\infty \right), \quad (55)$$

which meet the specified limit $\lim_{h\to 0} \epsilon_n = 0$ and since $\lim_{h\to 0} y_n(t_n) = y_n$. Then, the composite method in eq. (31) is convergent and the global truncation error order is $O\left(h^{2k-1}\right)$. □

6. Numerical examples

This section presents some well-established linear and non-linear ODEs to demonstrate how accurately the arising BVMs in eq. (13) perform. The methods presented herein are A-stable. The computations have been done using our written code in MATLAB 2010*a* [48].

Problem 1. Consider the non-linear system of equations solved by Wu-Xia [45]

$$\begin{matrix} y_1' = -1002 y_1 + 1000 y_2^2, & y_1(0) = 1 \\ y_2' = y_1 - y_2(1 + y_2), & y_2(0) = 1 \end{matrix}, \; y(t) = \begin{pmatrix} e^{-2t} \\ e^{-t} \end{pmatrix}, \quad (56)$$

with stiffness ratio 1002. It is clear from the results display in Table 3 that the HOBVLMM3 performs better in accuracy for different step sizes $h = \{0.02, 0.008\}$when compared with those in [20, 45]. The accuracy obtained from the new schemes improves that from ODE15s on this stiff problem. This is the case in general for all the problems solved.

Problem 2. The moderately stiff equations is considered in Jia-Xang and Jiao-Xun[12]

$$\begin{matrix} y' = \begin{pmatrix} -1 & -10 \\ 10 & -1 \end{pmatrix} y, \quad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \\ y(t) = \begin{pmatrix} e^{-t}\cos(10t) \\ e^{-t}\sin(10t) \end{pmatrix} \end{matrix}. \quad (57)$$

This system is moderately stiff with the stiffness ratio 1. This example is solved using the HOBVLMM3 in the interval $0 < t \le 20$. From Table 4, the HOBVLMM3 shows better performance compared to, the BDF of Gear [3] and the BVM in [20] of order $p = 5$ as the computations continues to the final point $t \in [0, 20]$. At dimension of $N = 125$ our methods produces superior accuracy to the other methods in [3, 20] even at the same order $p = 5$.

Problem 3. The linear stiff equation by Brugnano and Trigiante [19] is solved

$$\begin{matrix} y_1' = -21y_1 & 19y_2 & -20y_3 \\ y_2' = 19y_1 & -21y_2 & 20y_3 \\ y_3' = 40y_1 & -40y_2 & -40y_3 \end{matrix}; \quad y(0) = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad (58)$$

with the exact solution given as

$$y(t) = \begin{pmatrix} \frac{e^{-2t}}{2} + \frac{e^{-40t}}{2}(\cos(40t) + \sin(40t)) \\ \frac{e^{-2t}}{2} - \frac{e^{-40t}}{2}(\cos(40t) + \sin(40t)) \\ e^{-40t}(\cos(40t) - \sin(40t)) \end{pmatrix}.$$

The system in eq. (58) has stiffness ratio 28.5. In Table 5 the results of the HOBVLMM of order 3, 5 and 7 are displayed and compared with generalized backward differentiation formulas(GBDF) of order 3, 5 and 7 in [19] respectively. The new schemes demonstrate superior accuracy compared to the generalized backward differentiation formulas presented in [19]. The numerical order of convergence is defined as

$$\begin{matrix} rate = \log_2 \left(\frac{\max_{1<i<3} |y_i(t) - y_{i,h}| / |y_{i,h}|}{\max_{1<i<3} |y_i(t) - y_{i,\frac{h}{2}}| / |y_{i,\frac{h}{2}}|} \right) \\ i = 1, \cdots, 3; \quad 0 < t \le 1. \end{matrix} \quad (59)$$

Table 3: Maximum absolute error, error$_i$ = (max | $y_i - y(t_i)$ |) for Problem (1), $t = 1$.

Method	p	h	N	error$_1$	error$_2$
HOBVLMM3	5	0.02	50	2.12×10^{-13}	2.06×10^{-13}
[20]	5	0.02	50	3.20×10^{-12}	3.02×10^{-12}
HOBVLMM3	5	0.008	125	3.40×10^{-15}	2.51×10^{-15}
[20]	5	0.008	125	3.88×10^{-14}	3.10×10^{-14}
[45]	7	0.002	500	2.56×10^{-07}	8.02×10^{-8}
Ode15s				8.97×10^{-5}	1.23×10^{-4}

Table 4: Numerical result for Problem (2), error$_i$=(max | $y_i - y(t_i)$ |), $i = 1, 2$.

Method	p	h	N	t	$Error_1$	$Error_2$
HOBVLMM3	5	0.04	125	10	1.85×10^{-8}	8.01×10^{-8}
HOBVLMM3	5	0.04	125	20	1.45×10^{-13}	5.91×10^{-13}
[3]		0.04	122	5	3.8×10^{-4}	
			247	10	2.3×10^{-5}	
			497	20	1.8×10^{-9}	
[20]	5	0.04	125	5	8.33×10^{-6}	1.32×10^{-6}
			250	10	1.13×10^{-7}	1.36×10^{-8}
			500	20	8.19×10^{-12}	6.30×10^{-12}
Ode15s				10	9.52×10^{-6}	6.94×10^{-6}
Ode15s				20	5.75×10^{-6}	9.65×10^{-6}

Table 5: Maximum relative error for Problem (3) in the interval $0 < t \leq 1$.

h	HOBVLMM2 $k = 2, p = 3$	Rate	GBDF3 $k = 3, p = 3$	Rate	HOBVLMM3 $k = 3, p = 5$	Rate
1.0×10^{-2}	1.02×10^{-2}	(−)	2.52×10^{-2}	(−)	2.93×10^{-3}	(−)
5.0×10^{-3}	1.35×10^{-3}	(2.91)	3.62×10^{-3}	(2.80)	1.69×10^{-4}	(4.11)
2.5×10^{-3}	1.11×10^{-4}	(3.61)	4.90×10^{-4}	(2.88)	4.46×10^{-6}	(4.72)
1.25×10^{-3}	1.04×10^{-5}	(3.41)	7.21×10^{-5}	(2.76)	8.31×10^{-8}	(5.74)
6.25×10^{-4}	8.06×10^{-7}	(3.69)	9.71×10^{-6}	(2.89)	1.37×10^{-9}	(5.92)
h	**GBDF5 $k = 5, p = 5$**	**Rate**	**HOBVLMM4 $k = 4, p = 7$**	**Rate**	**GBDF7 $k = 7, p = 7$**	**Rate.**
1.0×10^{-2}	2.83×10^{-3}	(−)	7.81×10^{-4}	(−)	1.18×10^{-3}	(−)
5.0×10^{-3}	2.92×10^{-4}	(3.27)	5.43×10^{-6}	(7.16)	1.38×10^{-5}	(6.42)
2.5×10^{-3}	1.36×10^{-5}	(4.42)	4.16×10^{-8}	(7.02)	1.07×10^{7}	(7.00)
1.25×10^{-3}	5.04×10^{-7}	(4.26)	2.16×10^{-10}	(7.58)	1.07×10^{-9}	(6.64)
6.25×10^{-4}	1.70×10^{8}	(4.89)	1.26×10^{-12}	(7.41)	9.40×10^{12}	(6.84)

Problem 4. The Van der Pol problem

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= \epsilon(1 - y_1^2)y_2 - y_1, \end{aligned} \tag{60}$$

in [4] with initial value $y_0 = (2, 0)^T$, stepsize $h = 0.001$, $\epsilon = 10^2$. In Figure 4, we show the graph of the solution using HOBVLMM3 at integration $t = 500$. It was observed that the numerical solution of the HOBVLMM3 coincide with the MATLAB ODE15s in Figure 4.

Problem 5. The following chemistry problem was considered by Ismail and Ibrahim [50]

$$\begin{aligned} y_1' &= -0.03y_2 - 1000y_1y_2 - 2500y_1y_3; & y_1 &= 0 \\ y_2' &= -0.03y_2 - 1000y_1y_2; & y_2 &= 1 \\ y_3' &= -2500y_1y_3; & y_3 &= 1, \end{aligned} \tag{61}$$

with the theoretical result given as: $y(2) = \Big(-0.361693316989 \times 10^{-5}, 0.9815029948230, 1.018493388244\Big)^T$.

In Table 6, numerical results for the HOBVLMM3 are shown alongside a comparison to the step-by-step schemes

Table 6: The error results for Problem 5.

y_i	HOBVLMM3	Hojjati [50]	Ismail [49]	Error in ODE15s
y_1	0.67×10^{-19}	0.14×10^{-18}	0.82×10^{-10}	0.28×10^{-12}
y_2	0.85×10^{-14}	0.23×10^{-13}	0.61×10^{-5}	0.16×10^{-5}
y_3	0.71×10^{-13}	0.19×10^{-12}	0.57×10^{-5}	0.54×10^{-5}

Table 7: Comparison of solution for Problem (6), $h = 0.01$.

Methods	$T = 100$	$T = 200$	$T = 350$
HOBVLMM2	0.004707782756726	0.003111380131181	0.000837114241846
HOBVLMM3	0.004707781796265	0.003111379179628	0.000837113548213
HOBVLMM4	0.004707621528423	0.003111220398316	0.000837113543916
ODE15s	0.004707784149776	0.003111428986111	0.000837857170665

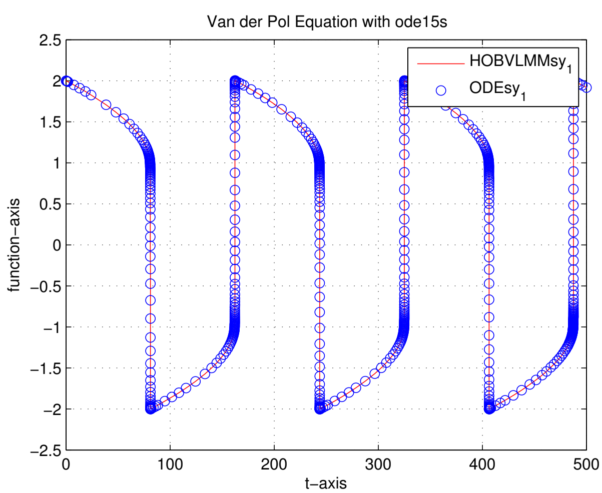

Figure 4: Solution for Problem 4 using HOBVLMM3.

from Hojjati *et al.* [50], Ismail [49] and MATLAB ODE15s [48]. It is shown from Table 6 that the HOBVLMM3 produce more accurate results than the methods in [49, 50]. The proposed method have the advantage of generating the solution simultaneously and this approach show a significant gain in efficiency over the compared in IVMs.

Problem 6. The stiff equations considered by Hairer and Wanner [4]

$$\begin{array}{rcll} y_1' &=& -a_1y_1 + a_2y_2 + a_3y_3 + 0.0007, & y_1 = 1\\ y_2' &=& a_1y_1 - a_4y_2, & y_2 = 0\\ y_3' &=& -a_5y_3 + a_2y_4 + a_6y_5, & y_3 = 0\\ y_4' &=& a_3y_2 + a_1y_3 - a_7y_4, & y_4 = 0\\ y_5' &=& -a_8y_5 + a_2y_6 + a_2y_7, & y_5 = 0\\ y_6' &=& -a_9y_6y_8 + a_{10}y_4 + a_1y_5 - a_2y_6 + a_{10}y_7, & y_6 = 0\\ y_7' &=& a_9y_6y_8 - a_{11}y_7, & y_7 = 0\\ y_8' &=& -a_9y_6y_8 + a_{11}y_7, & y_8 = 0.0052 \end{array} \quad (62)$$

with $a_1 = 1.71$, $a_2 = 0.43$, $a_3 = 8.32$, $a_4 = 8.75$, $a_5 = 10.03$, $a_6 = 0.035$, $a_7 = 1.12$, $a_8 = 1.745$, $a_9 = 280$, $a_{10} = 0.69$, $a_{11} = 1.81$. The scheme HOBVLMM of order 3, 5, and 7 is applied to problem 6 and the maximum error (max $| y_i - y_i(t) |$) is obtained by subtracting Output solution of the HOBVLM from the Output solution of ODE15s at various time $T = (100, 200, 300)$ in Table 7.

7. Conclusion

Conclusively, this paper has presented the HOBVLMM in eq. (13) for the numerical solution of the ODEs in eq. (1). The scheme possesses high-order for the same step number as that of extended backward differentiation formulas of Cash [6] and smaller error constant. The stability plots of HOBVLMM in eq. (13) for $k = 1, \cdots, 25$ have been presented in Figure (2) and (3). These newly derived schemes are $O_{k,k-1}$−stable and $A_{k,k-1}$−stable. The HOBVLMM in eq. (13) for $k = 2$, 3 and 4 has been implemented on some stiff problems herein. Compared to the step-by-step initial value LMMs in eq. (2), these methods offer the dual benefits of high order p and A-stability advantages similar to those of BVMs. Finally, we have obtained herein improved accuracies when compared to some standard existing methods.

Data availability

No data was used in the study.

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