Convergence Analysis of Modified Variable Step Block Backward Differentiation Formulae

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ABSTRACT:
This paper analyses the convergence of modified variable step block backward differentiation formulae (MVS-BBDF) method. We study the conditions for the method to be convergence and also investigate the order of the method. This method is proven to be of order four and consistent since it satisfies the conditions of consistency. To prove the validity of the method, the numerical experiments are carried out on stiff ordinary differential equations (ODEs) problem. The efficiency of the proposed method is compared with ODE solver in Matlab which are ode15s and ode23s. The results obtained prove that the proposed method has better performance as compared to ode15s and ode23s.

Keywords: Backward Differentiation Formulae, Block Backward Differentiation Formulae, Convergence, Order, Ordinary Differential Equations, Stiff Ordinary Differential Equations.

I. INTRODUCTION
In a scientific problem, a differential equation is usually accompanied by auxiliary conditions that (together with the differential equation) specify the unknown function precisely [1]. Basically, dynamical real-life problems may be formulated as a mathematical model either as a system of ordinary differential equations (ODEs) or partial differential equations (PDEs) [2].
Most people have some physical understanding of heat transfer due to its presence in many aspects of our daily life. Within mathematics, ODE plays an important role in the calculus variations, where optimal trajectories must satisfy the Euler equations, or in optimal control problems, where they satisfy the Pontryagin maximum principle. In both cases, one is led to boundary value problems for ODEs [3].

Moreover, differential equations with auxiliary conditions are known as an initial value problem (IVP). IVP of ODE may be linear or nonlinear, first-order or higher-order, and homogeneous or nonhomogeneous. A general form of a single differential equation of the first order accompanying an auxiliary condition is as follows

$$\frac{dx(t)}{dt} = f(t, x(t)), \quad x(t = a) = b$$

(1)

where $t$ is time and $t = a$ is the initial instant in time. $\frac{dx(t)}{dt}$ is denoted as the first derivative while $f(t, x(t))$ is denoted as derivative function. The solution to (1) is the function to $x(t)$. This function must satisfy an initial condition at $t = a, x(a) = b$.

The solution to a differential equation is the function that satisfies the differential equation and also satisfies certain initial conditions on the function. In solving a differential equation analytically, we usually find a general solution containing arbitrary constants and then evaluate the arbitrary constant so that the expression agrees with the initial conditions [4]. A special problem arising in the numerical solution of ODE is stiffness [5]. A stiff equation is a result of phenomena with widely differing time scales. Certain physical systems are sometimes modelled by differential equations for which the eigenvalues vary widely in magnitude [6].

To date, many methods have been established in order to find the solution for the IVP of stiff ODE problems, such as block backward differentiation formula (BBDF) method proposed by [7]. The block method has proven its advantages in producing less computational effort because it manages to compute more than one solution value per step using back values in the previous block when compared to the reduction method. Therefore, the problems in this paper are solved using one of the BBDF method, namely MVS-BBDF. It is proven in [8] that MVS-BBDF is stable for solving stiff ODEs where all the step size ratios (1, 2 and 5/9) satisfy the zero-stable and $A$-stable conditions.

Convergence is the requirement that the approximations generated by the method approach the actual solution as the step size goes to zero [5]. The numerical methods are converged if the numerical solutions approach the exact solution [9]. We use the definition and theorem given in [5] to define the convergence and consistency of linear multistep method (LMM).
**Definition 1** The LMM is convergent if,

\[ \lim_{n \to \infty} y_n = y(x), \quad h = \frac{x-a}{n}, \quad \text{for any arbitrary point } x \in [a, b] \]

**Theorem 1** The LMM is convergent if and only if it is consistent and zero stable.

Consistency is defined as the requirement that the differential equation used by the method to be equivalent to the differential equation as the step size goes to zero.

**Definition 2** The LMM is said to be consistent provided its error order \( p \) satisfies \( p \geq 1 \).

It can be shown that this implies that the first and second characteristic polynomials fulfil \( p(1) = 0, p'(1) = \sigma(1) \).

**Definition 3** The LMM is said to be consistent if

\[ \max_{k \leq n < N} \frac{t_n}{h} \to 0 \text{ as } h \to 0, \text{ provided } t_n \neq hy'. \]

Since BBDF method is a class of LMM, we use the same definition of convergence for LMM to define the convergence for our method.

**II. ORDER OF MVS-BBDF METHOD**

The order of MVS-BBDF method is discussed in this section using the definition of order for LMM. The multistep method uses the approximation values at more than one previous value to approximate the subsequent value. It can be written as a linear combination of the value of the solution and the value of the function at previous points. In this paper, we focused on MVS-BBDF method where the formulae is as below

\[ \begin{bmatrix} y_{n+1} \\ y_{n+2} \end{bmatrix} = \begin{bmatrix} \frac{1}{10}y_{n-2} - \frac{3}{5}y_{n-1} + \frac{9}{5}y_n \\ -\frac{3}{25}y_{n-2} + \frac{16}{25}y_{n-1} - \frac{36}{25}y_n \end{bmatrix} + \begin{bmatrix} \frac{6}{5}hf_{n+1} - \frac{3}{10}y_{n+2} \\ \frac{48}{25}y_{n+1} + \frac{12}{25}hf_{n+2} \end{bmatrix} \]

(2)

The general form of LMM is

\[ \sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j} \]

(3)

where \( k \) is the number of steps used in multistep, \( h \) is the step size, \( \alpha_j \) and \( \beta_j \) are constant with the conditions

\[ \alpha_k = 1 \text{ and } |\alpha_0| + |\beta_0| \neq 0. \]
Then, we obtain the general form of MVS-BBDF method in (3) as

$$\sum_{j=0}^{k} \alpha_j y_{n+2-j} = h \sum_{j=0}^{k} \beta_j f_{n+2-j}$$  

(4)

Define the LMM (3) associated with the linear difference operator \(L\).

$$L(y(x); h) = \sum_{j=0}^{k} \left[ \alpha_j y(x + jh) - h \beta_j y'(x + jh) \right]$$

(5)

where \(y(x)\) is an arbitrary function, continuously differentiable on \([a,b]\). Expanding the function \(y(x+jh)\) and its derivative \(y'(x+jh)\) as Taylor Series about \(x\). Thus, the equation becomes

$$L = \left[ y(x); h \right] = C_0 y(x) + C_1 h y(x) + C_2 h^2 y^2(x) + C_3 h^3 y^3(x) + \ldots + C_q h^q y^q(x)$$

(6)

where \(C_q\) are constants.

**Definition 4** The difference operator (6) and the associated linear multistep method (3) are said to be of order \(q\) if: \(C_0 = C_1 = \ldots = C_q = 0, \ C_{q+1} \neq 0\).

The constant \(C_q\) is defined in terms of the coefficients \(\alpha_j\) and \(\beta_j\) as follows

$$C_0 = \sum_{j=0}^{k} \alpha_j = \alpha_1 + \alpha_2 + \ldots + \alpha_k$$

$$C_1 = \sum_{j=0}^{k} (j \alpha_j - \beta_j) = \alpha_1 + 2 \alpha_2 + 3 \alpha_3 + \ldots + k \alpha_k - (\beta_0 + \beta_1 + \ldots + \beta_k)$$

$$C_2 = \sum_{j=0}^{k} \left( \frac{j^2 \alpha_j}{2} - j \beta_j \right) = \frac{1}{2} \left[ \alpha_1 + 2^2 \alpha_2 + 3^2 \alpha_3 + \ldots + k^2 \alpha_k \right] - (\beta_1 + 2 \beta_2 + \ldots + k \beta_k)$$

$$\ldots$$

$$C_q = \sum_{j=0}^{k} \left( \frac{j^q \alpha_j}{q!} - \frac{j^{q+1} \beta_j}{(q+1)!} \right) = \frac{1}{q!} \left[ \alpha_1 + 2^q \alpha_2 + 3^q \alpha_3 + \ldots \right] - \frac{1}{(q-1)!} \left[ \beta_1 + 2^{q-1} \beta_2 + 3^{q-1} \beta_3 + \ldots \right]$$

(7)
Given the linear difference operator $L$ associated with our method in (2) defined by

$$L(y(x); h) = \sum_{j=0}^{4} \left[ A_j y(x + jh) - h B_j y'(x + jh) \right]$$

(8)

where $C_q$ are constant column matrices. Equation (2) can also be expressed in matrix form as

$$h \begin{pmatrix} 0 & 0 & f_{n-3} & 0 & 0 \\ 0 & 0 & f_{n-2} & 0 & 0 \\ 0 & 0 & f_n & 0 & 0 \\ 0 & 0 & f_{n+1} & 0 & 0 \\ 0 & 0 & f_{n+2} & 0 & 0 \end{pmatrix} \begin{pmatrix} y_{n-3} \\ y_{n-2} \\ y_n \\ y_{n+1} \\ y_{n+2} \end{pmatrix} = \begin{pmatrix} -1 & 10 & 0 \\ 3 & 5 & -9 \\ 16 & 36 & 25 \\ 15 & -48 & 1 \end{pmatrix} \begin{pmatrix} y_{n-1} \\ y_n \\ y_{n+1} \\ y_{n+2} \end{pmatrix}$$

(9)

From equation (9), let

$$A_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad A_1 = \begin{pmatrix} -1 \\ 10 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 3 \\ 5 \end{pmatrix}, \quad A_3 = \begin{pmatrix} 16 \\ 36 \end{pmatrix}, \quad A_4 = \begin{pmatrix} 15 \\ -48 \end{pmatrix}, \quad A_5 = \begin{pmatrix} 1 \\ 10 \end{pmatrix}$$

$$B_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad B_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad B_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad B_3 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad B_4 = \begin{pmatrix} 6 \\ 5 \end{pmatrix}, \quad B_5 = \begin{pmatrix} 0 \\ 12 \end{pmatrix}$$

For this case, the values for $C_q$ are as below

$$C_0 = \sum_{j=0}^{5} A_j = 0,$$

$$C_1 = \sum_{j=0}^{5} (j A_j - B_j) = 0,$$

$$C_2 = \sum_{j=0}^{5} \left( \frac{j^2 A_j}{2!} - j B_j \right) = 0,$$

$$C_3 = \sum_{j=0}^{5} \left( \frac{j^3 A_j}{3!} - \frac{j^2 B_j}{2!} \right) = 0,$$

$$C_4 = \sum_{j=0}^{5} \left( \frac{j^4 A_j}{4!} - \frac{j^3 B_j}{3!} \right) = 0,$$

$$C_5 = \sum_{j=0}^{5} \left( \frac{j^5 A_j}{5!} - \frac{j^4 B_j}{4!} \right) = \begin{pmatrix} 3 \\ -50 \\ 12 \end{pmatrix} \neq \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

(10)
Since \( C_0 = C_1 = C_2 = 0, C_3 = 0, C_4 = 0 \) and \( C_5 \neq 0 \), from definition 1, this method is of order 4 and we can call the method as modified block backward differentiation formula of order 4.

III. CONVERGENT OF MVS-BBDF METHOD

**Theorem 2** The necessary and sufficient conditions for the linear multistep method of Equation (2) to be convergent are that it must be consistent and zero-stable.

Proof: See [10].

III.I CONSISTENCY OF MVS-BBDF METHOD

**Definition 5** A LMM (2) is said to be consistent if it has order \( p \geq 1 \). The method is consistent if and only if

\[
\sum_{j=0}^{k} \alpha_j = 0 \quad \text{and} \quad \sum_{j=0}^{k} j\alpha_j = \sum_{j=0}^{k} \beta_j \quad (11)
\]

See [10].

From the definition (2), we find the values of \( \sum_{j=0}^{5} A_j, \sum_{j=0}^{5} jA_j \) and \( \sum_{j=0}^{5} B_j \) below

\[
\sum_{j=0}^{5} A_j = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 10 \\ -15 \\ 15 \\ -16 \\ 16 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}
\]

\[
\sum_{j=0}^{5} jA_j = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + 1 \begin{bmatrix} 1 \\ -3 \\ 3 \\ -5 \\ 5 \\ 1 \end{bmatrix} + 2 \begin{bmatrix} 3 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 6 \\ 0 \\ 0 \\ 0 \end{bmatrix}
\]

\[
\sum_{j=0}^{5} B_j = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + 1 \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + 3 \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}
\]

(12)

Since the order of our method is four, which is \( \geq 1 \) as well as \( \sum_{j=0}^{5} A_j = 0 \) and \( \sum_{j=0}^{5} jA_j = \sum_{j=0}^{5} B_j \), therefore we can say that MVS-BBDF method is consistent.
III.11 ZERO STABILITY OF MVS-BBDF METHOD

**Definition 6** The LMM (2) is said to be zero stable if no root of the first characteristic polynomial \( p(r) \) has a modulus greater than one, and if every root with unit modulus is simple.

Apply method in (2) to the test equation, \( f = y' = \lambda \) and thus gives the stability polynomial as follows

\[
R(t; H) = \frac{197}{125} t^4 - \frac{153}{125} t^3 - \frac{9}{25} t^2 + \frac{1}{125} t - \frac{42}{25} t^4 H + \frac{72}{125} t^4 H^2
\]

(13)

\[
- \frac{252}{125} t^3 H - \frac{18}{125} t^2 H
\]

Proof: See [8].

To obtain zero stability, replace \( H = h\lambda = 0 \) to the stability polynomial in equation (13). Thus, we yield

\[
R(t; 0) = \frac{197}{125} t^4 - \frac{153}{125} t^3 - \frac{9}{25} t^2 + \frac{1}{125} t
\]

(14)

To obtain the roots, solve \( t \) in the equation (14). Therefore, we have the values of \( t \) as 1, 0.0207917599 and -0.2441420137. From definition 3, we can say that MVS-BBDF method is zero-stable since it satisfies the condition of zero-stability where all the roots are less than or equal to 1.

Consequently, the necessary conditions to be consistent have been fulfilled by the method in (2). Hence, the method shown in (2) is consistent.

**IV. RESULTS AND DISCUSSIONS**

In order to validate the efficiency of the proposed method, we provide three problems, found in [4], [11], and [12] in the numerical experiments.

**Problem 1** :

\[
y' = -1000y + 3000 - 2000e^{-x}, \quad x \in [0, 20]
\]

subject to the initial condition

\[
y(0) = 0
\]
with the exact solution
\[ y(x) = 3 - 0.998e^{-1000x} - 2.002e^{-x} \]
with eigenvalue
\[ \lambda = -100 \]

**Problem 2:**
\[ y' = -1000(y - 1), \quad x \in [0, 10] \]
subject to the initial condition
\[ y(0) = 2 \]
with the exact solution
\[ y(x) = e^{-1000x} + 1 \]
with eigenvalue
\[ \lambda = -1000 \]

**Problem 3:**
\[ y_1' = 998y_1 + 1998y_2 \]
\[ y_2' = -999y_1 - 1999y_2, \quad x \in [0, 20] \]
subject to the initial condition
\[ y_1(0) = 1, \quad y_2(0) = 0 \]
with the exact solution
\[ y_1(x) = 2e^{-x} - e^{-1000x} \]
\[ y_2(x) = -e^{-x} + e^{-1000x} \]
with eigenvalue
\[ \lambda = -1, -1000 \]
The notations below are used in the following tables and figures.

<table>
<thead>
<tr>
<th>Notation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MVS-BBDF</td>
<td>Modified variable step block backward differentiation formulae method</td>
</tr>
<tr>
<td>TSs</td>
<td>Total steps taken during the computation of approximate solution</td>
</tr>
<tr>
<td>TOL</td>
<td>Tolerance limit</td>
</tr>
<tr>
<td>MAXE</td>
<td>Maximum error</td>
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Table 1. Comparison results for Problem 1

<table>
<thead>
<tr>
<th>Problem</th>
<th>Method</th>
<th>TOL</th>
<th>TSs</th>
<th>MAXE</th>
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</thead>
<tbody>
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<td></td>
<td></td>
<td>$10^{-4}$</td>
<td>56</td>
<td>1.5807e-006</td>
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<td></td>
<td></td>
<td>$10^{-6}$</td>
<td>135</td>
<td>9.9454e-007</td>
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<tr>
<td></td>
<td>ode15s</td>
<td>$10^{-2}$</td>
<td>40</td>
<td>8.4000e-003</td>
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<td></td>
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<td>93</td>
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<td></td>
<td></td>
<td>$10^{-6}$</td>
<td>165</td>
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<tr>
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<td>ode23s</td>
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<td></td>
<td></td>
<td>$10^{-6}$</td>
<td>1193</td>
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Table 2. Comparison results for Problem 2

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<th>TSs</th>
<th>MAXE</th>
</tr>
</thead>
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Table 3. Comparison results for Problem 3

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<th>MAXE</th>
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<td>10^{-6}</td>
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Figure 1. Efficiency curves MVS-BBDF and Matlab’s ODE solvers for Problem 1

Figure 2. Efficiency curves MVS-BBDF and Matlab’s ODE solvers for Problem 2
Figure 3. Efficiency curves MVS-BBDF and Matlab’s ODE solvers for Problem 3

Figure 4. Total steps curves for Problem 1

Figure 5. Total steps curves for Problem 2
From the results obtained, Tables 1-3 and Fig. 1-6 show that MVS-BBDF method gave a better accuracy where the value of maximum error produced is the smallest when compared to ode15s and ode23s. In addition, the proposed method also produced less number of total steps for all of the problems considered.

V. CONCLUSION
From the analysis of the convergence and order of MVS-BBDF, it is proven that MVS-BBDF method is of order four method and consistent since it satisfied all the conditions of consistency. In addition, we have also shown the efficiency of the method by comparing our method with Matlab’s ODE solver, ode15s and ode23s. By comparing them, we found that MVS-BBDF method showed better performances in terms of accuracy and the number of total steps. In conclusion, MVS-BBDF method is suitable for solving stiff ODE problems.

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REFERENCES
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