

A Fourth Order Modified Block Backward Differentiation Formula for System of Stiff Initial Value Problems.

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Abstract

Abstract: This paper presents a fourth order Modified Block Backward Differentiation Formula (MBBDF) for the numerical solution of stiff ordinary differential equations. This is achieved by constructing a Modified Backward Differentiation formula (MBDF) with continuous coefficients together with the additional methods from its first derivative and are combined to form a single block that simultaneously provide the approximate solutions for the stiff Initial Value Problems (IVPs). The stability property of the (MBBDF) is discussed and the performance of the method is demonstrated on some numerical examples to show the accuracy and efficiency advantages of the method.

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1.0 Introduction

The first order initial value problem (IVP) of the form

$$y' = f(t, y), \quad y(t_0) = y_0, \quad (1)$$

on the interval $I = [t_0, T_n]$, where $t \in R$, $y: R \rightarrow R^m$ and $f: R \times R^m \rightarrow R^m$, m is the dimensionality of the system, The equation (1) is stiff if its Jacobian has eigenvalues that satisfies the condition

$$\frac{\max |\operatorname{Re}(\lambda_i)|}{\min |\operatorname{Re}(\lambda_i)|} > 1,$$

with $\operatorname{Re}(\lambda_i) < 0$. The quest for a good numerical method for the solution of (1) with good accuracy and wide stability region has been the concern of numerical analyst. Since 1959 after the discovery of the Backward Differential Formula (BDF) by Curtis and Hirschfelder [1], which is generally written in the form

$$\sum_{j=0}^{k-1} \alpha_j y_{n+j} = h\beta_k f_{n+k} \quad (2)$$

for the solution of stiff IVPs, several other methods have been proposed for efficiently solving (1), (see Butcher [2], Cash [3], Gear [4], Enright[5], Hairer and Wanner [6], Hosseini and Hojjati [7], Kap[8], Kohfeld and Thompson [9], Lambert

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[10], and Skelboe and Christiansen [11]). In Brugnano and Trigiante [12], a generalized Backward Differentiation Formula (GBDF) with special stability properties was proposed and implemented as a boundary value method, while in Keiper and Gear [13], a zero-stable generalized BDF of order 7 was proposed and used to solve differential-algebraic equations.

The development of continuous approximations for initial value problems (IVPs) has been the subject of growing interest due to the fact that continuous methods enjoy certain advantages, such as the potential for them to provide defect control (see Enright [5]) as well as having the ability to generate additional methods Onumanyi et al [14], Jator [15], Akinfenwa et al. [17], [18]).

In this paper a fourth order Modified Backward Differentiation Formula (MBDF) with continuous coefficients in the form

$$Y(t) = \sum_{j=0}^{k-1} \alpha_j(t) y_{n+j} - h(\beta_{k-1}(t) f_{n+k-1} + \beta_k(t) f_{n+k}), \quad (3)$$

is developed with additional method combined as block method known as MBBDF for the numerical solution of stiff systems (1). Where h is the step size $\alpha_j(t)$, $\beta_{k-1}(t)$, $\beta_k(t)$ are continuous coefficient that must be determined and n is the grid index. The continuous coefficients enable us to develop the main method and additional method which are combined as a single block method to provide the approximate solution y_{n+i} , $i = 1, 2, \dots, k$ to the exact $y(t_{n+i})$, $i = 1, 2, \dots, k$ of (1) in the first block making use of only the initial value given in the problem as the starting value. It would be observe that block methods were first introduced by Milne [16] and since then various block methods including continuous ones have been developed (see [17], [18], [19], [20], [21] and the references therein). It is important to observe that the fourth order MBBDF preserves the Runge-kutta traditional advantage of being self-starting and is more efficient, since it requires only three function evaluation per integration step.

The rest of this paper is presented as follows. In section 2 we derive the MBBDF by obtaining a continuous representation $Y(t)$ for the exact solution $y(t)$ which is used to generates a main discrete method and additional methods for solving (1), in section 3 the order of accuracy and stability property of the methods are discussed, section 4 is the computational aspect MBBDF algorithm. Numerical examples are given in section 5 to show the accuracy and efficiency advantages. Finally,

the conclusion of the paper is discussed in Section 6.

2.0 Derivation of MBBDF

In this section, we develop the MCBDF with the additional methods derived from its first derivative combined to form the MBBDF on the interval from t_n to $t_{n+3} = t_n + 3h$ where h is the chosen step-length. In particular, we assume that the exact solution $y(t)$ on the interval $[t_n, t_{n+3}]$ is locally represented by $Y(t)$ given by

$$Y(t) = \sum_{j=0}^{p+q-1} b_j \varphi_j(t) \quad (4)$$

b_j are unknown coefficients to be determined, and $\varphi_j(t)$ are polynomial basis function of degree $p + q - 1$. such that the number of interpolation points p and the number of distinct collocation points q are respectively chosen to satisfy $p = k$, $q > 0$. The proposed method is thus constructed by specifying the following parameters: $\varphi(t_{n+j}) = t_{n+j}^j$, $j = 0, \dots, 4$ $p = 3$, $q = 2$, and $k = 3$.

by imposing the following conditions

$$\sum_{j=0}^4 b_j t_{n+i}^j = y_{n+i} \quad , \quad i = 0, 1, 2 \quad , \quad (5)$$

$$\sum_{j=0}^4 j b_j t_{n+i}^{j-1} = f_{n+i} \quad , \quad i \in 2, 3 \quad , \quad (6)$$

assuming that $y_{n+j} = Y(t_n + ih)$ denote the numerical approximation to the exact solution $y(t_{n+j})$, $f_{n+j} = Y'(t_n + ih)$ denote the approximation to $y'(t_{n+j})$, n is the grid index. It should be noted that equation (5) and (6) lead to a system of five equations which is solved by matrix inversion to obtain the coefficients b_j $j = 0, 1, \dots, 4$. The MBDF with continuous coefficients is then obtained by substituting these values of b_j into equation (4). After some algebraic computation, the method yields the expression in the form

$$Y(t) = \alpha_0(t)y_n + \alpha_1(t)y_{n+1} + \alpha_2(t)y_{n+2} - h(\beta_2(t)f_{n+2} + \beta_3(t)f_{n+3}) \quad , \quad (7)$$

where $\alpha_j(t)$, $j=0, 1, 2$, $\beta_2(t)$, $\beta_3(t)$ are continuous coefficients that are given as

$$\alpha_0(t) = \frac{(h-t+t_n)(2h-t+t_n)^2(17h-5t+5t_n)}{68h^4} \quad , \quad \alpha_1(t) = \frac{(t-t_n)(2h-t+t_n)^2(24h-7t+7t_n)}{17h^4} \quad ,$$

$$\alpha_2(t) = \frac{(t-t_n)(h-t+t_n)(228h^2 - 23(t+t_n)^2 + 143h(-t+t_n))}{68h^4} \quad ,$$

$$\beta_2(t) = \frac{(t-t_n)(h-t+t_n)(2h-t+t_n)(39h+11(-t+t_n))}{34h^3} \quad ,$$

$$\beta_3(t) = -\frac{(t-t_n)(h-t+t_n)(2h-t+t_n)^2}{17h^3} \quad ,$$

Equation (7) is then used to generate the main discrete MBDF by evaluating at point $t = t_{n+3}$ to yield

$$y_{n+3} = -\frac{1}{17}y_n + \frac{9}{17}y_{n+1} + \frac{9}{17}y_{n+2} + \frac{18}{17}f_{n+2} + \frac{6}{17}f_{n+3} \quad (8)$$

Differentiating (7) with respect to t we have

$$Y'(t) = \frac{1}{h}(\overline{\alpha_0(t)}y_n + \overline{\alpha_1(t)}y_{n+1} + \overline{\alpha_2(t)}y_{n+2} - h(\overline{\beta_2(t)}f_{n+2} - \overline{\beta_3(t)}f_{n+3})) \quad , \quad (9)$$

where $\overline{\alpha_j(t)}$, $j=0, 1, 2$, $\overline{\beta_2(t)}$, and $\overline{\beta_3(t)}$ are continuous coefficients.

The additional methods are obtained by evaluating (9) at points $t = \{t_{n+}, t_{n+1}\}$ to obtain

$$f_n = -\frac{39}{17}y_n + \frac{96}{17}y_{n+1} - \frac{57}{17}y_{n+2} + \frac{39}{17}f_{n+2} - \frac{4}{17}f_{n+3} \quad (10)$$

$$f_{n+1} = -\frac{3}{17}y_n - \frac{24}{17}y_{n+1} + \frac{27}{17}y_{n+2} - \frac{14}{17}f_{n+2} + \frac{1}{17}f_{n+3} \quad (11)$$

the methods (9),(10), and (11), are combined to give the MBBDF as

$$\left. \begin{aligned} f_n &= -\frac{39}{17}y_n + \frac{96}{17}y_{n+1} - \frac{57}{17}y_{n+2} + \frac{39}{17}f_{n+2} - \frac{4}{17}f_{n+3} \\ f_{n+1} &= -\frac{3}{17}y_n - \frac{24}{17}y_{n+1} + \frac{27}{17}y_{n+2} - \frac{14}{17}f_{n+2} + \frac{1}{17}f_{n+3} \\ y_{n+3} &= -\frac{1}{17}y_n + \frac{9}{17}y_{n+1} + \frac{9}{17}y_{n+2} + \frac{18}{17}f_{n+2} + \frac{6}{17}f_{n+3} \end{aligned} \right\} \quad (12)$$

3.0 Order of accuracy and Stability of MBBDF

The modified block backward differentiation formulae can be represented by a matrix finite difference equation in block form as.

$$A^{(1)}Y_{\overline{\omega}+1} = A^{(0)}Y_{\overline{\omega}} + hB^{(1)}F_{\overline{\omega}+1} + hB^{(0)}F_{\overline{\omega}} \quad (13)$$

Where

$$\begin{aligned} Y_{\overline{\omega}+1} &= (y_{n+1}, y_{n+2}, y_{n+3})^T, \\ Y_{\overline{\omega}} &= (y_{n-2}, y_{n-1}, y_n)^T, \\ F_{\overline{\omega}+1} &= (f_{n+1}, f_{n+2}, f_{n+3})^T, \\ F_{\overline{\omega}} &= (f_{n-2}, f_{n-1}, f_n)^T \end{aligned}$$

$$\overline{\omega} = 0, 1, 2, \dots \text{ and } n = 0, k, \dots, N - 3$$

And the matrices $A^{(1)}$, $A^{(0)}$, $B^{(1)}$ are 3 by 3 matrices whose entries are given by the coefficients of (12) given as

$$\begin{aligned} A^{(1)} &= \begin{pmatrix} \frac{24}{17} & -\frac{27}{17} & 0 \\ -\frac{96}{17} & \frac{57}{17} & 0 \\ \frac{17}{17} & -\frac{9}{17} & 1 \end{pmatrix} & A^{(0)} &= \begin{pmatrix} 0 & 0 & -\frac{3}{17} \\ 0 & 0 & -\frac{39}{17} \\ 0 & 0 & \frac{1}{17} \end{pmatrix}, & B^{(1)} &= \begin{pmatrix} -1 & -\frac{14}{17} & \frac{1}{17} \\ 0 & \frac{39}{17} & -\frac{4}{17} \\ 0 & \frac{18}{17} & \frac{6}{17} \end{pmatrix}, \\ B^{(0)} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned}$$

The local truncation error associated with the MBDF can be defined to be the linear difference operator

$$L[y(t); h] = \sum_{j=0}^2 \alpha_j y_{n+j} - h(\beta_2 f_{n+2} + \beta_3 f_{n+3}) \quad (14)$$

Assuming that $y(t)$ is sufficiently differentiable, we can write the terms in (14) as a Taylor series expression of $y(t_{n+j})$ and $f(t_{n+j}) = y'(t_{n+j})$ as

$$y(t_{n+j}) = \sum_{j=0}^{\infty} \frac{(jh)^m}{m!} y^{(m)}(t_n) \text{ and } y'(t_{n+j}) = \sum_{j=0}^{\infty} \frac{(jh)^m}{m!} y^{(m+1)}(t_n) \quad (15)$$

Substituting (14) into the equations in (12) we obtain the expression

$$L [y(t_n) ; h] = C_0 y(t) + C_1 h y'(t) + C_2 h^2 y''(t) + \dots + C_s h^m y^{(m)}(t) + \dots$$

Where the constant C_m , $m = 0, 1, 2, \dots$ are given as follows:

$$C_0 = \sum_{j=0}^2 \alpha_j$$

$$C_1 = \sum_{j=1}^2 j \alpha_j - \beta_2 - \beta_3 + \gamma_l$$

$$C_2 = \frac{1}{2!} \sum_{j=1}^2 j \alpha_j - 2\beta_2 - 3\beta_3 + \gamma_l$$

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$$C_m = \frac{1}{m!} \left[\sum_{j=1}^2 j^m \alpha_j - m 2^{m-1} \beta_2 - m 3^{m-1} \beta_3 + m l^{m-1} \gamma_l \right]$$

Where $\gamma_k = 0$, $\gamma_l = 1$, $l = 0, 1$

The method in (12) is said to have a maximal order of accuracy m if

$$L [y(t_n) ; h] = C_{m+1} h^{m+1} y^{(m+1)}(t_n) + O(h^{m+2})$$

And

$$C_0 = C_1 = C_2 \dots C_m = 0, \quad C_{m+1} \neq 0 \tag{16}$$

Therefore, C_{m+1} is the error constant and $C_{m+1} h^{m+1} y^{(m+1)}(t_n)$ the principal local truncation error at the point t_n .

Therefore, the values of the error constants calculated for MBBDF (12) is given as:

$$\left(-\frac{13}{170}, \frac{19}{170}, \frac{-1}{51} \right)^T \text{ with order } (4, 4, 4)^T \text{ and T is the transpose}$$

3.1 Zero Stability

The zero stability of the method is concerned with the stability of the difference system in the limit as h tends to zero.[18] Thus, as $h \rightarrow 0$ the difference system (13) tends to

$$A^{(1)} Y_{\overline{\omega}+1} = A^{(0)} Y_{\overline{\omega}}$$

Whose first characteristics polynomial $\rho(R)$ given by

$$\rho(R) = \det[RA^{(1)} - A^{(0)}] = \frac{72}{17} R^2 (1 - R) \tag{17}$$

The block method (12) is zero stable for $\rho(R)=0$ and satisfies $|R_j| \leq 1$, $j = 1, \dots, 3$, and for those roots with $|R_j| = 1$, the multiplicity does not exceed 1. hence the modified block BDF methods with continuous coefficients are zero stable.

3.2 Consistency and Convergence

We note that the block method (12) is consistent as it has order $p > 1$. Since the block method (12) is zero stable and Convergence = zero stability + consistency. Hence the method (12) converges.

3.3 Linear Stability

The stability properties of the block formulae (12) is discussed and determined through the application to the test equation

$$y' = \lambda y, \quad \lambda < 0 \tag{18}$$

applying (12) to (18) yields

$$Y_{\overline{w}+1} = Q(z)Y_{\overline{w}}, \tag{19}$$

where $Q(z)$ is the amplification matrix with $z = h\lambda$ given by

$$Q(z) = (A^{(1)} + zB^{(1)})^{-1} \cdot (A^{(0)} + B^{(0)})$$

The matrix $Q(z)$ has eigenvalues $(\xi_1, \xi_2, \xi_3) = (0, 0, \xi_3)$ where the dominant eigenvalue ξ_3 is a rational function of z given by

$$\xi_3(z) = \frac{12 + 18z + 11z^2 + 3z^3}{12 - 18z + 11z^2 - 3z^3} \tag{20}$$

which is the stability function of the methods (12).

From (20) the usual property of A-stability which requires that for all $z = h\lambda \in C^-$ and $\zeta_3(z) < 0$ is obtained. The absolute stability region S associated with the block method (12) is the set

$S = \{z = h\lambda : \text{for that } z \text{ where the roots of the stability function (20) are of moduli less than one}\}$. In the spirit of Hairer and Wanner [5], the stability region S is presented in white colour which corresponds to the fourth order modified block BDF (20). Clearly, from the Figure 1, it is obvious that the method is A- stable, since it has no pole of the stability function (20) represented by the plus sign in the left half complex plane and also satisfies the L- stability condition that

$$\lim_{z \rightarrow \infty} \text{Re}(z) = 0 \quad \text{where } z = h\lambda.$$

Therefore, the method is L-Stable.

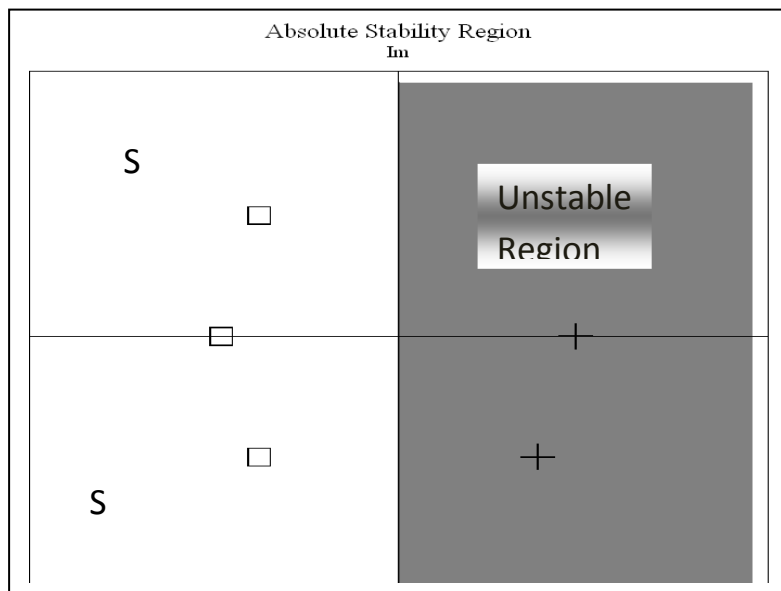


Figure 1. Absolute stability region

4.0 Computational aspect MBBDF

The newly derived method is implemented more efficiently as a 3-step block numerical integrators for (1) to simultaneously obtain the approximations $(y_{n+1}, y_{n+2}, y_{n+3})^T$ without requiring back values or predictors taking $n = 0, 3, \dots, N - 3$ over sub-intervals $[t_0, t_3], \dots, [t_{N-3}, t_N]$. For example $n = 0, \varpi = 0, (y_1, y_2, y_3)^T$, are simultaneously obtained over the sub-interval $[t_0, t_3]$, as y_0 is known from the initial value problem (1). $n=3, \varpi = 1, (y_4, y_5, y_6)^T$ are simultaneously obtained over the sub-interval $[t_3, t_6]$ as y_3 is known from previous block and so on. Hence, the sub-intervals do not over-lap. The computations were carried out using our written code in Matlab. It should be noted that for linear problems, the code used Gaussian elimination and for nonlinear problems, the Newton's method is used

5.0 Numerical Example

This section deals with some numerical examples, executed in MATLAB language with double precision arithmetic, which illustrate the result derived in the previous sections.

Example 5.1 Consider the stiff system of initial value problem which has been solved by Zarina et.al. [20]:

$$\begin{aligned} y_1'(t) &= 198y_1 + 199y_2 & , & & y_1(0) &= 1 \\ y_2'(t) &= -398y_1 - 399y_2 & , & & y_2(0) &= -1 \end{aligned} \quad 0 \leq t \leq 10$$

The exact solution is

$$y_1(t) = -y_2(t) \quad , \quad y_2(t) = -e^{-x}$$

Eigenvalues: $\lambda_1 = -1$, $\lambda_2 = -200$

The result in [21] is reproduced in table 1 and compared with the new method (12) and that obtained with the continuous block BDF (CBBDF)[17] for $k=3$. It can be seen in Table 1 that the result obtained for MBBDF is superior to those of BBDF and CBBDF for the same number of steps

Table 1 Comparison of methods for Example 5.1. Max error = $\max_{1 \leq i \leq NS} |y_i - y(t_i)|$

h	Number of steps	Zarina et-al [21] BBDF Max error	CBBDF k=3 [17] Max error	New method (12) MBBDF k=3 Max error
10^{-2}	333	1.07308×10^{-2}	4.61670×10^{-8}	4.675416×10^{-11}
10^{-3}	3333	1.10060×10^{-3}	4.60608×10^{-11}	1.160183×10^{-14}
10^{-4}	33333	1.10333×10^{-4}	6.60305×10^{-13}	9.140693×10^{-14}

Example 5.2 Consider also another stiff system which has also been solved by Alberdi et.al. [21]:

$$\begin{aligned}
 y_1'(t) &= -0.1y_1 - 49.9y_2, & y_1(0) &= 2 \\
 y_2'(t) &= -50y_2, & y_2(0) &= 1 \\
 y_3'(t) &= 70y_2 - 120y_3, & y_3(0) &= 2
 \end{aligned}$$

The stiffness ratio of this problem is 1 : 200 and the exact solution is

$$y_1(t) = e^{-50t} + e^{-0.1t}, \quad y_2(t) = e^{-50t}, \quad y_3(t) = e^{-50t} + e^{-120t}$$

In Table 2 the results obtained by [21] is reproduced and compared with that obtained using the MBBDF. From Table 2. It can be seen that the MBBDF is superior to that of EBDF, EBPDF and ENPDF as given in Alberdi et.al. [21]

Table 2 Comparison of methods for Example 5.2 for 50 steps. Error = $|y_i - y(t_i)|$

t	y_i	Error in EBDF k=4	Error in EBPDF k=4	Error in ENPDF k=4	Error in ENDF k=4	Error in MBBDF k=3
5	y_1	0.26×10^{-2}	0.24×10^{-2}	0.24×10^{-2}	0.22×10^{-2}	0.54×10^{-3}
	y_2	0.26×10^{-2}	0.24×10^{-2}	0.24×10^{-2}	0.22×10^{-2}	0.54×10^{-3}
	y_3	0.23×10^{-2}	0.19×10^{-2}	0.20×10^{-2}	0.15×10^{-2}	0.26×10^{-2}
10	y_1	0.87×10^{-8}	0.80×10^{-8}	0.79×10^{-8}	0.70×10^{-8}	0.73×10^{-11}
	y_2	0.23×10^{-9}	0.18×10^{-9}	0.15×10^{-9}	0.10×10^{-9}	0.73×10^{-11}
	y_3	0.61×10^{-9}	0.48×10^{-9}	0.54×10^{-9}	0.38×10^{-9}	0.17×10^{-11}
20	y_1	0.81×10^{-8}	0.74×10^{-8}	0.73×10^{-8}	0.65×10^{-8}	0.15×10^{-13}
	y_2	0.56×10^{-18}	0.38×10^{-18}	0.20×10^{-18}	0.17×10^{-18}	0.15×10^{-21}
	y_3	0.15×10^{-17}	0.95×10^{-18}	0.12×10^{-17}	0.48×10^{-18}	0.46×10^{-21}

Example 5.3 Further example is the nonlinear stiff system proposed by Kaps [8], and used in [19] by P. Chartier. The results in [19] for k=3 is reproduced in Table 3 and compared with CBBDF[17] and that of the MBBDF given in equation (12)

$$\begin{cases} y_1' = -(\epsilon^{-1} + 2)y_1 + \epsilon^{-1}y_2^2, & y_1(0) = 1 \\ y_2' = y_1 - y_2 - y_2^2, & y_2(0) = 1 \end{cases} \quad 0 \leq t \leq T$$

the smaller ϵ is, the more serious the stiffness of the system. The exact solution is

$$y_1(t) = y_2^2(t), \quad y_2(t) = e^{-t}$$

In Table 3 it is obvious that the number of correct digit denoted by Δ , is greater for MBBDF than those in CBBDF and $M(3, r_3)$

$$\Delta = -\text{Log}_{80} \left\| \frac{y_i(T) - y_{n,1}}{y_{n,1}} \right\|_{\infty} \quad (21)$$

Table 3: A comparison of methods for Example 5.3. Number of correct digits Δ , $T=4$ and $\epsilon = 10^{-8}$

Method	$h = 1/4$	$h = 1/8$	$h = 1/16$	$h = 1/32$	$h = 1/64$	$h = 1/128$	$1/256$
$MCBBDF_3$	3.37	4.62	5.81	7.02	8.22	9.43	13.29
$CBBDF_3$	1.92	2.79	3.46	4.53	5.42	5.74	7.10
$M(3, r_3)$ of P. Chartier [19]	1.06	1.88	2.75	3.64	4.53	5.43	6.33

6.0 Conclusion

We have proposed a fourth order MBBDF for the solution of system of stiff IVPs. The method is self-starting and provides good accuracy. Numerical examples using the three step MBBDF showed that the method is accurate and efficient as evident in Table 1, 2, 3.

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