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Numerical Solution of Extended Block Backward Differentiation Formulae for Solving Stiff ODEs

S. A. M. Yatim, Z. B. Ibrahim, K.I. Othman and M. B. Suleiman

Abstract—**Existing Block Backward Differentiation Formulae (BBDF) of different orders are collected based on their competency and accuracy in solving stiff ordinary differential equations (ODEs). The strategy to fully utilize the formulae is optimized using variable step variable order approach. The improved performances in terms of accuracy and computation time are presented in the numerical results with different sets of test problems. The comparison is made between the proposed method and MATLAB's suite of ordinary differential equations (ODEs) solvers namely ode15s and ode23s.**

Index Terms— **Numerical Analysis, Initial Value Problem, Ordinary Differential Equations, Stiff ODEs, BBDF methods**

I. INTRODUCTION

MOTIVATED by applied problems arise from physical, biological and physical phenomenon, there are numbers of researches commenced to devise effective and very accurate methods to solve stiff ODEs [1]. Gear's method which is associated with backward differentiation formula (BDF) in [2] has presented promising results in certain point of comparison. Some popular codes based on BDF include LSODE and VODE. The most recent code associated with BDF is called MEBDF presented in [3] has also discussed its performance on a large set of stiff tests problems. Because of a broad class of problems occurred in applied sciences [4]-[7], the methods are developed giving rigorous results in terms of accuracy and computation time.

The study of numerical methods for solving stiff initial value problems for ODEs is said to have reached a certain maturity. Many in recent papers have tried to describe and compare some of the best codes available [8]. Because of that, there now exist some excellent codes which are both efficient and reliable for solving these particular classes of problems. A crucial component in developing an efficient ODE solver is by taking into accounts their accuracy, rate of convergence, and computation time. This is of great importance in situation example in astronomy, when long-term, very accurate and reliable numerical solution is sought.

The study on BBDF was first introduced in [9] demonstrates the competency of computing concurrent solution values at different points. Consequently, study in [10] is extended in a way that the accuracy is improved by increasing the order of the method up to order 5 [11]. Thus, BBDF of order 3 to 5 are collected and we introduce variable step variable order approach to its strategy in choosing the stepsize. We are interested to compare the numerical results obtained with stiff ODEs solvers available in Matlab; ODE15s and ODE23s.

The problems considered in this paper are for the numerical solution of the initial value problem,

$$y' = f(x, y) \quad (1)$$

with given initial values $y(a) = y_0$ in the given interval $x \in [a, b]$.

II. DERIVATION OF EXTENDED BLOCK BACKWARD DIFFERENTIATION FORMULAE METHOD

A. Construction of Extended Block Backward Differentiation Formulae method

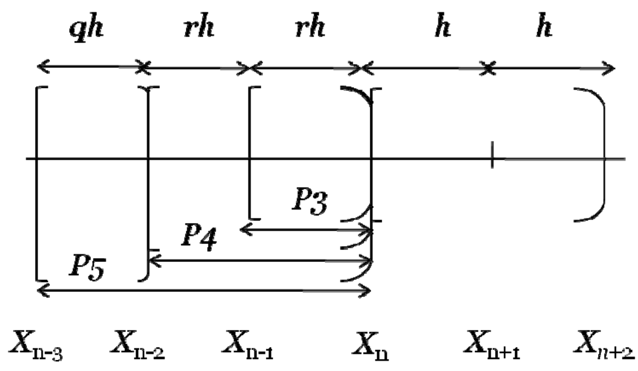

Fig 1. Extended BBDF method of order *(P3-P5)*

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Two values of y_{n+1} and y_{n+2} were computed simultaneously in block by using earlier blocks with each block containing a maximum of two points (Fig 1). The orders of the method (*P3*, *P4* and *P5*) are distinguished by the number of backvalues contained in total blocks. The ratio distance between current (x_n) and previous step (x_{n-1}) is represented as r and q in Fig 1. In this paper, the step size is given selection to decrease to half of the previous steps, or increase up to a factor of 1.9. For simplicity, q is assigned as 1, 2 and 10/19 for the case of constant, halving and increasing the step size respectively. The zero stability is achieved for each of these cases and explained in the next section.

We find approximating polynomials $P_k(x)$, by means of a *k*-degree polynomial interpolating the values of *y* at given points are $(x_{n-3,}y_{n-3})$, $(x_{n-2,}y_{n-2})$, $(x_{n-1,}y_{n-1})$ …, (x_{n+2}, y_{n+2}).

$$P_k = \sum_{j=0}^{k} y(x_{n+1-j}).L_{k,j}(x) \qquad (2)$$

where

$$L_{k,j}(x) = \prod_{\substack{i=0 \\ i\neq j}}^{k} \frac{(x - x_{n+1-i})}{(x_{n+1-j} - x_{n+1-i})}$$

for each $j = 0,1,...,k$

The interpolating polynomial of the function $y(x)$ using Lagrange polynomial in (2) gives the following corrector for the first point y^{p}_{n+1}, and second point y^{p}_{n+2} . The resulting Lagrange polynomial for each order was given as follows:

For Extended BBDF of order *P3* ($P = 3$)

$$\begin{aligned} P(x) &= P(x_{n+1} + sh) \\ &= \frac{(r+1+s)(s+1)(s)}{2r+4} y_{n+2} + \frac{(r+1+s)(s+1)(s-1)}{-1-r} y_{n+1} \\ &+ \frac{(r+1+s)(s-1)(s)}{2r} y_n + \frac{(1+s)(s-1)(s)}{-r(-1-r)(-r-2)} y_{n-1} \end{aligned} \qquad (3)$$

For Extended BBDF of order *P4* ($P = 4$)

$$\begin{aligned} P(x) &= P(x_{n+1} + sh) \\ &= \frac{(2r+1+s)(r+1+s)(1+s)(s)}{2(2r+2)(r+2)} y_{n+2} \\ &+ \frac{(2r+1+s)(r+1+s)(1+s)(s-1)}{-(2r+1)(r+1)} y_{n+1} \\ &+ \frac{(2r+1+s)(r+1+s)(s)(s-1)}{4r^2} y_n \\ &+ \frac{(2r+1+s)(1+s)(s)(s-1)}{-r^2(-r-1)(-r-2)} y_{n-1} \\ &+ \frac{(r+1+s)(1+s)(s)(s-1)}{2r^2(-2r-1)(-2r-2)} y_{n-2} \end{aligned} \qquad (4)$$

For Extended BBDF of order *P5* ($P = 5$)

$$\begin{aligned} P(x) &= P(x_{n+1} + sh) \\ &= \frac{(q+2r+1+s)(2r+1+s)(r+1+s)(1+s)s}{2(q+2r+2)(2r+2)(r+2)} y_{n+2} \\ &+ \frac{(q+2r+1+s)(2r+1+s)(r+1+s)(1+s)(s-1)}{-(q+2r+1)(2r+1)(r+1)} y_{n+1} \\ &+ \frac{(q+2r+1+s)(2r+1+s)(r+1+s)s(s-1)}{4(q+2r)r^2} y_n \\ &+ \frac{(q+2r+1+s)(2r+1+s)(1+s)s(s-1)}{-r^2(q+r)(-r-1)(-r-2)} y_{n-1} \\ &+ \frac{(q+2r+1+s)(r+1+s)(1+s)s(s-1)}{2qr^2(-2r-1)(-2r-2)} y_{n-2} \\ &+ \frac{(2r+1+s)(r+1+s)(1+s)s(s-1)}{-q(-q-r)(-q-2r)(-q-2r-1)(-q-2r-2)} y_{n-3} \end{aligned} \qquad (5)$$

By substituting $s = 0$ and $s = 1$ gives the corrector for the first and second point respectively. Therefore by letting $r = 1, q = 1$, $r = 2, q = 2$ and $r = 1, q = 10/19$ we produced the following equations for the first and second point of Extended BBDF.

Extended BBDF of order *P3* ($P = 3$)

When $r = 1, q = 1$

$$y_{n+1} = 2hf_{n+1} - \frac{2}{3} y_{n+2} + 2y_n - \frac{1}{3} y_{n-1}$$

$$y_{n+2} = \frac{6}{11} hf_{n+2} + \frac{18}{11} y_{n+1} - \frac{9}{11} y_n + \frac{2}{11} y_{n-1}$$

When $r = 2, q = 2$

$$y_{n+1} = 3hf_{n+1} - \frac{9}{8} y_{n+2} + \frac{9}{4} y_n - \frac{1}{8} y_{n-1}$$

$$y_{n+2} = \frac{4}{7} hf_{n+2} + \frac{32}{21} y_{n+1} - \frac{4}{7} y_n + \frac{1}{21} y_{n-1}$$

When $r = 1, q = 10/19$

$$y_{n+1} = \frac{29}{19} hf_{n+1} - \frac{841}{1824} y_{n+2} + \frac{841}{380} y_n - \frac{361}{480} y_{n-1}$$

$$y_{n+2} = \frac{48}{91} hf_{n+2} + \frac{4608}{2639} y_{n+1} - \frac{576}{455} y_n + \frac{6859}{13195} y_{n-1}$$

Extended BBDF of order *P4* ($P = 4$)

When $r = 1, q = 1$

$$y_{n+1} = \frac{6}{5} hf_{n+1} - \frac{3}{10} y_{n+2} + \frac{9}{5} y_n - \frac{3}{5} y_{n-1} + \frac{1}{10} y_{n-2}$$

$$y_{n+2} = \frac{12}{25} hf_{n+2} + \frac{48}{25} y_{n+1} - \frac{36}{25} y_n + \frac{16}{25} y_{n-1} - \frac{3}{25} y_{n-2}$$

When $r = 2, q = 2$

$$y_{n+1} = \frac{15}{8} hf_{n+1} - \frac{75}{128} y_{n+2} + \frac{225}{128} y_n - \frac{25}{128} y_{n-1} + \frac{3}{128} y_{n-2}$$

$$y_{n+2} = \frac{12}{23} hf_{n+2} + \frac{192}{115} y_{n+1} - \frac{18}{23} y_n + \frac{3}{23} y_{n-1} - \frac{2}{115} y_{n-2}$$

When $r = 1, q = 10/19$

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$$y_{n+1}=\frac{1131}{1292}hf_{n+1}-\frac{14703}{82688}y_{n+2}+\frac{1279161}{516800}y_n-\frac{183027}{108800}y_{n-1}+\frac{10469}{27200}y_{n-2}$$

$$y_{n+2}=\frac{1392}{3095}hf_{n+2}+\frac{89088}{40235}y_{n+1}-\frac{242208}{77375}y_n+\frac{198911}{77375}y_{n-1}-\frac{658464}{1005875}y_{n-2}$$

Extended BBDF of order *P5* ($P=5$)
When $r=1, q=1$

$$y_{n+1}=\frac{12}{13}hf_{n+1}-\frac{12}{65}y_{n+2}+\frac{24}{13}y_n-\frac{12}{13}y_{n-1}+\frac{4}{13}y_{n-2}-\frac{3}{65}y_{n-3}$$

$$y_{n+2}=\frac{60}{137}hf_{n+2}+\frac{300}{137}y_{n+1}-\frac{300}{137}y_n+\frac{200}{137}y_{n-1}-\frac{75}{137}y_{n-2}+\frac{12}{137}y_{n-3}$$

When $r=2, q=2$

$$y_{n+1}=\frac{105}{71}hf_{n+1}-\frac{3675}{9088}y_{n+2}+\frac{3675}{2272}y_n-\frac{1225}{4544}y_{n-1}+\frac{147}{2272}y_{n-2}-\frac{75}{9088}y_{n-3}$$

$$y_{n+2}=\frac{24}{49}hf_{n+2}+\frac{3072}{1715}y_{n+1}-\frac{48}{49}y_n+\frac{12}{49}y_{n-1}-\frac{16}{245}y_{n-2}+\frac{3}{343}y_{n-3}$$

When $r=1, q=10/19$

$$y_{n+1}=\frac{402}{449}hf_{n+1}-\frac{13467}{77228}y_{n+2}+\frac{13467}{7184}y_n-\frac{13467}{13021}y_{n-1}+\frac{4489}{8980}y_{n-2}\frac{7428297}{44792240}y_{n-3}$$

$$y_{n+2}=\frac{516}{1189}hf_{n+2}+\frac{177504}{79663}y_{n+1}-\frac{5547}{2378}y_n+\frac{59168}{34481}y_{n-1}-\frac{5547}{5945}y_{n-2}+\frac{7428297}{23102270}y_{n-3}$$

As similar to analysis for order of Linear Multistep Method (LMM) given in [12], we use the following definition to determine the order of Extended BBDF method.

Definition 3.1
The LMM [12] and the associated difference operator L defined by

$$L[z(x);h]=\sum_{k=0}^{j}[\alpha_k z(x+kh)-h\beta_k z'(x+kh)] \quad (6)$$

Are said to be of order p if $c_o=c_1=...=c_p=0$, $C_{p+1}\neq 0$. The general form for the constant C_q is defined as

$$C_q=\sum_{k=0}^{j}[k^q\alpha_k-\frac{1}{(q-1)!}k^{q-1}\beta_k]\ ,\quad q=2,3,...p+1 \quad (7)$$

Consequently, BBDF method can be represented in standard form by an equation $\sum_{j=0}^{k}A_j y_{n+j}=h\sum_{j=0}^{k}B_j f_{n+j}$ where A_j and B_j are r by r matrices with elements $a_{l,m}$ and $b_{l,m}$ for $l,m=1,2,...r$. Since Extended BBDF for variable order (P) is a block method, we extend the definition 3.2 in the form of

$$L[z(x);h]=\sum_{k=0}^{j}[A_k z(x+kh)-hB_k z'(x+kh)] \quad (8)$$

And the general form for the constant C_q is defined as

$$C_q=\sum_{k=0}^{j}[k^q A_k-\frac{1}{(q-1)!}k^{q-1}B_k]\ q=2,3,...p+1 \quad (9)$$

A_k is equal to the coefficients of y_k where $k=n=(P-2),...,n+1,n+2$ and $P=3,4,5$.

Throughout this section, we illustrate the effect of Newton-type scheme which in general form of

$$y^{(i+1)}_{n+1,n+2}-y^{(i)}_{n+1,n+2}=\frac{\left[(I-A)y^{(i)}_{n+1,n+2}-hBF(y^{(i)}_{n+1,n+2})-\xi\right]}{-\left[(I-A)-hB\frac{\partial F}{\partial y}(y^{(i)}_{n+1,n+2})\right]} \quad (10)$$

The general form of Extended BBDF method is

$$\left.\begin{aligned}y_{n+1}&=\alpha_1 hf_{n+1}+\theta_1 y_{n+2}+\psi_1\\ y_{n+2}&=\alpha_1 hf_{n+2}+\theta_1 y_{n+1}+\psi_2\end{aligned}\right\} \quad (11)$$

with ψ_1 and ψ_2 are the back values. By setting ,

$$I=\begin{bmatrix}1&0\\0&1\end{bmatrix},\ y_{n+1,n+2}=\begin{bmatrix}y_{n+1}\\y_{n+2}\end{bmatrix},,$$

$$B=\begin{bmatrix}\alpha_1&0\\0&\alpha_2\end{bmatrix},\ F_{n+1,n+2}=\begin{bmatrix}f_{n+1}\\f_{n+2}\end{bmatrix},\ \text{and}\ \xi_{n+1,n+2}=\begin{bmatrix}\psi_1\\\psi_2\end{bmatrix}$$

Equation (11) in matrix-vector form is equivalent to

$$(I-A)y_{n+1,n+2}=hBF_{n+1.n+2}+\xi_{n+1,n+2} \quad (12)$$

Equation (12) is simplified as

$$\hat{f}_{n+1,n+2}=(I-A)y_{n+1,n+2}-hBF_{n+1,n+2}-\xi_{n+1,n+2}=0 \quad (13)$$

Newton iteration is performed to the system $\hat{f}_{n+1,n+2}=0$, by taking the analogous form of (10) where $J_{n+1,n+2}=\left(\frac{\partial F}{\partial Y}\right)(Y^{(i)}_{n+1,n+2})$, is the Jacobian matrix of F with respect to Y. Equation (10) is separated to three different matrices denoted as

$$E_{1,2}^{(i+1)} = y_{n+1,n+2}^{(i+1)} - y_{n+1,n+2}^{(i)} \quad (14)$$

$$\hat{A} = (I - A) - hB\frac{\partial F}{\partial Y}(y_{n+1,n+2}^{(i)}) \quad (15)$$

$$\hat{B} = (I - A)y_{n+1,n+2}^{(i)} - hBF(y_{n+1,n+2}^{(i)}) - \xi_{n+1,n+2} \quad (16)$$

Two-stage Newton iteration works to find the approximating solution to (1) with two simplified strategies based on evaluating the Jacobian ($J_{n+1,n+2}$) and LU factorization of $\hat{A}$ [12].

B. *Order and stepsize selection*

The importance of choosing the step size is to achieve reduction in computation time and number of iterations. Meanwhile changing the order of the method is designed for finding the best approximation. Strategies proposed in [13] are applied in this study for choosing the step size and order. The strategy is to estimate the maximum step size for the following step. Methods of order *P*-1, *P*, *P*+1 are selected depending on the occurrence of every successful step. Consequently, the new step size h_{new} is obtained from which order produces the maximum step size.

The user initially will have to provide an error tolerance limit, TOL on any given step and obtain the local truncation error (LTE) for each iteration. The LTE is obtained from

$$LTE_k = y_{n+2}^{(P+1)} - y_{n+2}^{(P)}, \; P = 3,4,5$$

where $y_{n+2}^{(P+1)}$ is the $(P+1)$-th order method and $y_{n+2}^{(P)}$ is the k-th order method. By finding the LTEs, the maximum step size is defined as

$$h_{P-1} = h_{old} \times \left(\frac{TOL}{LTE_{P-1}}\right)^{\frac{1}{P}}, \quad h_P = h_{old} \times \left(\frac{TOL}{LTE_P}\right)^{\frac{1}{P+1}},$$

$$h_{P+1} = h_{old} \times \left(\frac{TOL}{LTE_{P+1}}\right)^{\frac{1}{P+2}}$$

Where h_{old} is the stepsize from previous block and $h_{\max}$ is obtained from the maximum stepsize given in above equations.

The successful step is dependent on the condition LTE<TOL. If this condition fails, the values of y_{n+1}, y_{n+2} are rejected, and the current step is reiterated with step size selection $(q = 2)$. On the contrary, the step size increment for each successful step is defined as

$h_{new} = c \times h_{\max}$ and if

$h_{new} > 1.9 \times h_{old}$ then $h_{new} = 1.9 \times h_{old}$

where c is the safety factor, p is the order of the method while h_{old} and h_{new} is the step size from previous and current block respectively. In this paper, c is set to be 0.8 so as to make sure the rejected step is being reduced.

III. Numerical Results

We carry out numerical experiments to compare the performance of Extended BBDF method with stiff ODE solvers in **MATLAB** mentioned earlier. These test problems are performed under different conditions of error tolerances – (a) 10^{-2}, (b) 10^{-4} and, (c) 10^{-6}

The test problems and solution are listed below

Problem 1

$$y' = -100(y - x) + 1 \quad y(0) = 1 \quad 0 \le x \le 10$$

With solution:

$$y(x) = e^{-100x} + x$$

Problem 2

$$y_1' = -1002y_1 + 1000y^2 \quad y_1(0) = 1 \quad 0 \le x \le 10$$

$$y_2' = y_1 - y_2(1 + y_2) \quad y_2(0) = 0$$

With solution:

$$y_1 = e^{-2x}$$

$$y_2 = e^{-x}$$

The abbreviations used in the following tables and figures are listed below:

TS	:	the total number of steps taken
TOL	:	the initial value for the local error estimate
MAXE	:	the maximum error
AVEE	:	the average error
MTD	:	the method used
TIME	:	the total execution time (seconds)

TABLE I
NUMERICAL RESULTS FOR PROBLEM (1).

TOL	MTD	TS	AVEE	MAXE	TIME
10^{-2}	Extended BBDF	21	2.9370e-005	2.8298e-004	0.0103
	ode15s	28	1.3000e-003	8.4000e-003	0.0313
	ode23s	19	1.0000e-003	4.5000e-003	0.1406
10^{-4}	Extended BBDF	48	1.0716e-006	3.2212e-006	0.0105
	ode15s	60	3.0358e-005	1.6621e-004	0.0156
	ode32s	42	1.1285e-004	2.5683e-004	0.0313
10^{-6}	Extended BBDF	164	1.6733e-008	3.1232e-008	0.0115
	ode15s	100	7.2564e-007	2.7506e-006	0.0313
	ode23s	143	7.3558e-006	1.2514e-005	0.0469

This paper considers the comparison of four different factors namely number of steps taken, average error, maximum error and computation time. From Table 1, among the three methods tested, our method, Extended BBDF method requires the shortest execution time, smallest maximum error and average error for each given tolerance level.

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TABLE II
NUMERICAL RESULTS FOR PROBLEM (2).

TOL	MTD	TS	AVEE	MAXE	TIME
10^{-2}	Extended BBDF	22	7.1459e-005	2.5736e-004	0.0106
	ode15s	29	9.0287e-004	5.2000e-003	0.0781
	ode23s	25	3.3626e-004	1.1000e-003	0.0781
10^{-4}	Extended BBDF	54	7.4173e-006	3.7659e-004	0.0111
	ode15s	55	1.7139e-005	8.5506e-005	0.1250
	ode32s	118	1.3783e-005	6.9774e-005	0.2031
10^{-6}	Extended BBDF	194	6.3429e-009	3.2882e-008	0.0143
	ode15s	197	2.1320e-007	1.0790e-006	0.2344
	ode23s	773	3.3163e-007	2.8081e-006	0.4531

Again by comparing four factors mentioned earlier, we can see Extended BBDF in Table 2 gives the least value of maximum error for every tolerance level except for TOL 10e-4. However, our method prevails in terms of average error for each given tolerance level. Extended BBDF once again requires the shortest execution time for each given tolerance level.

IV. CONCLUSION

The objective is met when Extended BBDF method outperformed ode15s and ode23s in term of average error as well as maximum error. In most of the cases, Extended BBDF has successfully managed to reduce the number of total steps taken. As for the computation time wise, it gave lesser values for all cases. Therefore, we can conclude that Extended BBDF can serve as an alternative solver for solving stiff ordinary differential equations.

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