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Fifth Order Variable Step Block Backward Differentiation Formulae for Solving Stiff ODEs

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***Abstract*—**The implicit block methods based on the backward differentiation formulae (BDF) for the solution of stiff initial value problems (IVPs) using variable step size is derived. We construct a variable step size block methods which will store all the coefficients of the method with a simplified strategy in controlling the step size with the intention of optimizing the performance in terms of precision and computation time. The strategy involves constant, halving or increasing the step size by 1.9 times the previous step size. Decision of changing the step size is determined by the local truncation error (LTE). Numerical results are provided to support the enhancement of method applied.

***Keywords*—**Backward differentiation formulae, block backward differentiation formulae, stiff ordinary differential equation, variable step size.

I. INTRODUCTION

WE consider the first order Ordinary Differential Equations (ODEs) in the form of

$$y' = f(x, y) \tag{1}$$

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

According to Cash [3], the rapid growth of the studies on the extension traditional method for solving ODEs have led to somewhat competition in deriving an efficient algorithms for solving stiff and non-stiff systems. Some of the earliest method that incorporated with BDF was proposed by Gear [7]. The later method evolved in many ways including Modified Extended Backward Differentiation Formulae (MEBDF) [4], and the most recent study is on producing block approximations $y_{n+1}, y_{n+2}, y_{n+3}, ..., y_{n+k}$ also known as Block Backward Differentiation Formulae (BBDF) [8]. Zarina *et. al* [8] has stated that the competency of computing concurrent solution values at different points has given BBDF an extra credit in saving computation time. Consequently, block approximations has been used in different methods but the idea is more or less similar, which is aimed to construct relatively better methods in producing better approximations provided that, a good computation time and average errors are maintained.

As far as this paper is concerned, we are interested to extend the study by Zarina *et. al* in [9] with a purpose to use every means to give a better accuracy with reduction of total steps and lesser computational time. Instead of increasing the step size by 1.6, it is changed to a factor of 1.9 and at the same time, the zero stability is ensured.

In the next section, we discuss the difference between the present paper and the one in [9], so that the significance of this paper is more apparent. The strategies and implementations are made different, hence we are able to see the trend of the result obtained.

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II. GENERAL FIFTH ORDER VARIABLE STEP BBDF FORMULATION

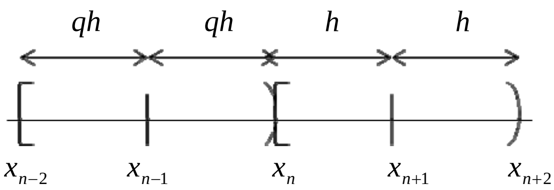

Fig. 1 2-point block method of variable step size

The step size ratio is defined as q, represents the distance between the current and previous $2qh$ step size block as in fig. 1. The step size is allowed to decrease down to half of the previous steps, and increase up to a factor of 1.9 so as to make sure the condition of zero stability is satisfied. Therefore, this paper considered the values of q as 1, 2 and 10/19. Since doubling the step size is zero unstable, the maximum allowable factor value, yet zero stable is taken as 1.9.

We find approximating polynomials $P_k(x)$ specifying certain point through which they must pass. By means of a *k*-degree polynomial interpolating, the values of *y* at given points are (x_{n-2}, y_{n-2}), (x_{n-1}, y_{n-1}),..., (x_{n+2}, y_{n+2}).

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

where

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

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Define $s = \dfrac{x - x_{n+1}}{h}$ to find the 4th interpolating polynomial for (2).

s is equated to 0 and 1 after the polynomial is differentiated with respect to s when $x = x_{n+1}$ and $x = x_{n+2}$ respectively.

For the full view of the equations obtained, please refer to [9].

Upon substituting $q = 1,2$ and $10/19$ into $p'(x_{n+1})$ and $P'(x_{n+2})$, we obtained the coefficients for points x_{n+1} and x_{n+2} as

For $q = 1$

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

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

For $q = 2$

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

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

For $q = 10/19$

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

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

The difference in the present paper can be seen in the alternative new sets of coefficients for the first and second points of the BBDF method. The selected values of q are taken to maintain zero stability and computational efficiency.

III. Implementation of Fifth Order Variable Step BBDF Method

In order to find the approximation solutions of y_{n+1} and y_{n+2} simultaneously in every step, we consider the application of a Newton-type scheme to some stiff equation. The general forms of the 2-point BBDF method are

$$\left.\begin{aligned} y_{n+1} &= \alpha_1 hf_{n+1} + \theta_1 y_{n+2} + \psi_1 \\ y_{n+2} &= \alpha_2 hf_{n+2} + \theta_2 y_{n+1} + \psi_2 \end{aligned}\right\} \quad (3)$$

with ψ_1 and ψ_2 are the back values.

Equation (3) in matrix-vector form is equivalent to

$$(I - A)Y_{n+1,n+2} = hBF_{n+1,n+2} + \xi_{n+1,n+2}$$

By letting

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, Y_{n+1,n+2} = \begin{bmatrix} y_{n+1} \\ y_{n+2} \end{bmatrix}, A = \begin{bmatrix} 0 & \theta_1 \\ \theta_2 & 0 \end{bmatrix},$$

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

The equation (3) is simplified as

$$\hat{f}_{n+1,n+2} = (I - A)Y_{n+1,n+2} - hBF_{n+1,n+2} - \xi_{n+1,n+2} \quad (4)$$

Newton iteration is performed to the system $\hat{f}_{n+1,n+2} = 0$, by taking the analogous form

$$Y^{(i+1)}_{n+1,n+2} - Y^{(i)}_{n+1,n+2} = -\left[(I - A) - hb\frac{\partial F}{\partial Y}(Y^{(i)}_{n+1,n+2})\right]^{-1}(I - A)Y^{(i)}_{n+1,n+2} - hBF(Y^{(i)}_{n+1,n+2}) - \xi_{n+1,n+2}$$

where $J_{n+1,n+2} = \dfrac{\partial F}{\partial Y}(Y^{(i)}_{n+1,n+2})$, is the Jacobian matrix of F with respect to Y.

A. Choosing step size

In order to reduce the computation time alongside with the iterations, three basic strategies are proposed for the step size adjustment. For each successful step, the step size remains constant $(q = 1)$ or increased by a factor of $1.9\,(q = 10/19)$. Inversely, when a fail step occurs, the next step size will be halved of the previous step size $(q = 2)$. The user initially will have to provide an error tolerance limit, TOL on any given step and obtain the LTE for each iteration. The LTE is obtained from

$$LTE = y^{(k+1)}_{n+2} - y^{(k)}_{n+2}, \quad k = 4.$$

where $y^{(k+1)}_{n+2}$ is the $(k+1)$ th order method and $y^{(k)}_{n+2}$ is the k th order method.

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

$$h_{new} = c \times h_{old} \times \left(\frac{TOL}{LTE}\right)^{\frac{1}{p}} \text{ and if}$$

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

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.

IV. Numerical Results

Two sets of stiff problems are tested in present paper for the purpose of elucidating the difference in numerical results obtained by using variable step of 2-point BBDF method. The test problem and solution are listed below

PROBLEM 1: $y' = -100(y - x) + 1$, $y(0) = 1$, $0 \le x \le 10$

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

Eigenvalue: $\lambda = -100$

Source: Gear, [7]

PROBLEM 2: $y_1' = -1002 y_1 + 1000 y^2$, $y_1(0) = 1$

$y_2' = y_1 - y_2(1 + y_2)$, $y_2(0) = 1$, $0 \le x \le 20$

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

$y_2 = e^{-x}$

Source: Kaps, [12]

The abbreviations used in the next table, are listed below:

TP : the test problem
TS : the total number of steps taken
TOL : the initial value for the local error estimate
FSs : the total number of failure steps
STs : the total number of successful steps
MAXE: the maximum error
STR : strategy in increasing the step size during the implementation of variable step 2-point BBDF
TIME : the total execution time (micro seconds)

TABLE I
NUMERICAL RESULT FOR PROBLEM (1) AND (2)

TP	TOL	STR	FSs	STs	TS	MAXE	TIME
1)	10^{-2}	1.6	0	26	26	1.20172e-04	1229
		1.9	0	21	21	9.91711e-05	1131
	10^{-4}	1.6	0	42	42	8.35132e-07	1346
		1.9	0	37	37	8.62759e-07	1339
	10^{-6}	1.6	0	86	86	1.02048e-08	1641
		1.9	0	85	85	6.63262e-09	1634
2)	10^{-2}	1.6	0	29	29	5.86134e-05	1570
		1.9	0	26	26	5.35937e-05	1465
	10^{-4}	1.6	0	53	53	2.84605e-06	1932
		1.9	0	51	51	3.03964e-06	1176
	10^{-6}	1.6	0	122	122	1.12154e-07	2777
		1.9	0	125	125	1.26618e-09	2718

V. Conclusion

For all problems tested, it shows that, even with a slight change in the step size selection, it managed to reduce the number of total steps taken in most of the cases. However, in terms of computation time wise, it gave lesser values for all cases.

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