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VARIABLE STEP BLOCK BACKWARD DIFFERENTIATION FORMULA FOR SOLVING FIRST ORDER STIFF ODEs

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Abstract— This paper focuses on the derivation of implicit 2-point block method based on Backward Differentiation Formulae (BDF) of variable step size for solving first order stiff initial value problems (IVPs) for Ordinary Differential Equations (ODEs). In a 2-point Block Backward Differentiation Formula (BBDF), two solution values are produced simultaneously. Plots of their regions of absolute stability for the method are also presented. The efficiency of the 2-point BBDF is compared with variable step variable order non block BDF (NBDF) method. Numerical results indicate that the resulting 2-point BBDF method outperform the NBDF method in both execution time and accuracy.

Keywords: Backward Differentiation Formulae, block, stiff.

I. INTRODUCTION

Many fields of application, notably in science and engineering, yield initial value problems involving systems of Ordinary Differential Equations (ODEs) and many of these problems are known as stiff ODEs. There have been various definitions of stiffness given in the literature with respect to the linear systems of first order equations,

$$\tilde{y}' = A\tilde{y} + \tilde{\phi}(x), \quad \tilde{y}(a) = \tilde{\eta}\,, \quad a \le x \le b \qquad (1.1)$$

where $\tilde{y}^T = (y_1, y_2, ..., y_s)$ and $\tilde{\eta}^T = (\eta_1, \eta_2, ..., \eta_s)$

For simplicity, we choose the definition of stiffness given by Lambert [7], which is as follows.

Definition: The linear systems (1.1) is said to be stiff if

(i) $\operatorname{Re}(\lambda_i) < 0, \quad i = 1,...,s$ and

(ii) $\max_i \left| \operatorname{Re}(\lambda_i) \right| \gg \min_i \left| \operatorname{Re}(\lambda_i) \right|$ where λ_i are the eigenvalues of *A*, and the ratio $\dfrac{\max_i \left|\operatorname{Re}(\lambda_i)\right|}{\min_i \left|\operatorname{Re}(\lambda_i)\right|}$ is called the stiffness ratio or stiffness index.

II. BLOCK METHOD FOR SOLVING ODEs

Among the earliest research on block methods was proposed by Shampine and Watts [10,13] with block implicit one-step methods, Chu and Hamilton [3] with multi-block methods, Voss and Abbas [12] with block predictor-corrector schemes. Other block methods are discussed by several researchers such as Houwen and Sommeijer [5] with block Runge-Kutta methods, Omar [9] and Majid [8] with block method based on Adams type formulas for solving nonstiff ODEs

Motivated by the fact that there are very few work been done in solving stiff ODEs using block method, we develop a variable step size block methods based on Backward Differentiation Formulas which will be called BBDF. In a 2-point BBDF, two solution i.e. y_{n+1} and y_{n+2} values are computed simultaneously. Hence, given the points y_{n-2}, y_{n-1} and y_n as backvalues, we derive a formula which defines the next block of approximations y_{n+1} and y_{n+2} simultaneously.

III. FORMULATION OF 2-POINT BBDF METHOD

In this section, we consider 2-point block methods for the numerical solution of ODEs

$$y' = f(x, y), \quad y(a) = y_0\,, \quad a \le x \le b\,. \qquad (3.1)$$

The step size of the computed block is 2*h* and the step size of the previous block is $2rh$ where r is the step size ratio (Refer Figure 3.1). In this case, the values considered were $r = 1$, $r = 2$ and $r = 5/8$ which corresponds respectively with constant step size, half the step size and increment of the step size by a factor of 1.6. We do not consider doubling the step size ($r = 0.5$) due to zero instability.

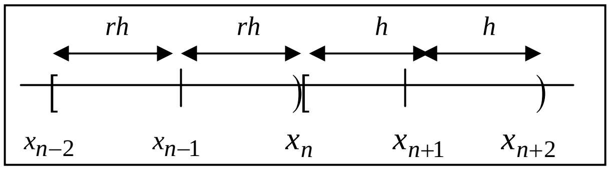


Figure 3.1: 2-point BBDF of variable step size

Consider the polynomial $P_k(x)$ of degree k which interpolates the values $y_n, y_{n-1}, ..., y_{n-k+1}$ of a function *f* at the interpolating points $x_n, x_{n-1}, ..., x_{n-k+1}$ in terms of Lagrange polynomial defined as follows:

$$P_k(x) = \sum_{j=0}^{k} L_{k,j}(x)\, f\left(x_{n+1-j}\right) \tag{3.2}$$

where

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

Define $s = \dfrac{x - x_{n+1}}{h}$ and replace $f(x,y)$ in (3.1) by polynomial (3.2). Differentiating the resulting polynomial once with respect to *s* at the point $x = x_{n+1}$ and evaluating at $s = 0$ gives the following

$$P'(x) = P'(x_{n+1}) = hf_{n+1} = \frac{1+2r^2+3r}{4(1+r)(2+r)} y_{n+2}$$
$$+\frac{2+3r}{(1+r)(1+2r)} y_{n+1} + \frac{-1-2r^2-3r}{4r^2} y_n + \frac{1+2r}{r^2(1+r)(2+r)} y_{n-1}$$
$$+\frac{-1-r}{4r^2\left(1+3r+2r^2\right)} y_{n-2} \tag{3.3}$$

Similarly, differentiating the resulting polynomial once with respect to *s* at the point $x = x_{n+2}$ and substituting $s = 1$ yields

$$P'(x) = P'(x_{n+2}) = hf_{n+2} = \frac{20+6r^2+24r}{4(1+r)(2+r)} y_{n+2}$$
$$-\frac{8+4r^2+12r}{(1+r)(1+2r)} y_{n+1} + \frac{4+2r^2+6r}{4r^2} y_n + \frac{-4-4r}{r^2(1+r)(2+r)} y_{n-1}$$
$$+\frac{4+2r}{4r^2\left(1+3r+2r^2\right)} y_{n-2} \tag{3.4}$$

On substituting $r = 1$, 2 , and r = 5/8 into (3.3) and (3.4) gives the coefficients for the first and second point of the BBDF method. These values of r are considered to ensure zero stability and computational efficiency.

(i) for $r = 1$

$$-\frac{1}{10} y_{n-2} + \frac{3}{5} y_{n-1} - \frac{9}{5} y_n + y_{n+1} + \frac{3}{10} y_{n+2} = \frac{6}{5} hf_{n+1}$$
$$\frac{3}{25} y_{n-2} - \frac{16}{25} y_{n-1} + \frac{36}{25} y_n - \frac{48}{25} y_{n+1} + y_{n+2} = \frac{12}{25} hf_{n+2}$$

(ii) for $r = 2$

$$-\frac{3}{128} y_{n-2} + \frac{25}{128} y_{n-1} - \frac{225}{128} y_n + y_{n+1} + \frac{75}{128} y_{n+2} = \frac{15}{8} hf_{n+1}$$
$$\frac{2}{115} y_{n-2} - \frac{3}{23} y_{n-1} + \frac{18}{23} y_n - \frac{192}{115} y_{n+1} + y_{n+2} = \frac{12}{23} hf_{n+2}$$

(iii) for $r = 5/8$

$$-\frac{208}{775} y_{n-2} + \frac{6912}{5425} y_{n-1} - \frac{13689}{6200} y_n + y_{n+1} + \frac{351}{1736} y_{n+2} = \frac{117}{124} hf_{n+1}$$
$$\frac{12544}{29875} y_{n-2} - \frac{53248}{29875} y_{n-1} + \frac{74529}{29875} y_n - \frac{2548}{1195} y_{n+1} + y_{n+2} = \frac{546}{1195} hf_{n+2}$$

Note that the above formula is in the similar form of a standard BDF. This allows us to store the coefficients of the *y* values and thus avoiding calculating the differentiation coefficients at each step but robust enough to allow for step size variation.

IV. STABILITY OF THE BBDF METHODS

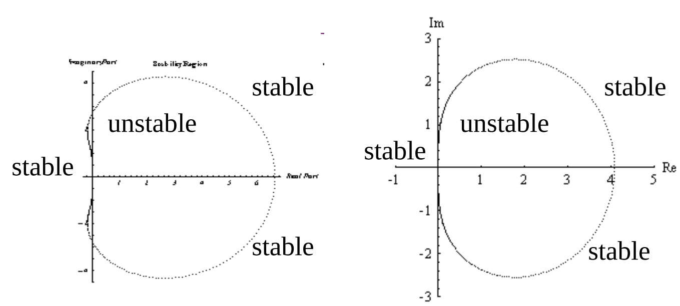
In this section, the stability properties of the proposed methods are analyzed to demonstrate their relevance in solving stiff problems. For the method to be of practical importance in solving stiff problems, it must posses at least almost *A*-stable property.

Definition: A numerical method is called *A*-stable if the whole of the left half plane, $\{z : \mathrm{Re}(z) \le 0\}$ is contained in the region $\{z : |R(z)| \le 1\}$ where $R(z)$ is called the stability polynomial of the method.

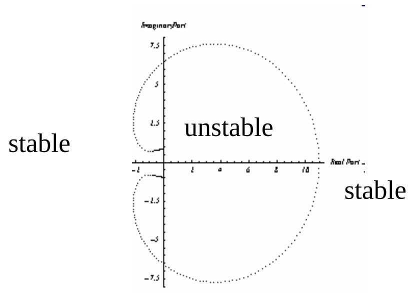
The linear stability properties of the methods are determined through application of the standard linear test problem

$$y' = \lambda y, \quad \lambda < 0 \text{ , } \lambda \text{ complex.} \tag{4.1}$$

The boundary of the stability region is given by the set of points determined by $t = e^{i\theta}$, $0 \le \theta \le 2\pi$. for which $|t| < 1$. Below we present the stability region *R* which corresponds to the 2- point BBDF method drawn in the $h\lambda$ plane



r = 1 r = 2



r = 5/8

The stability region which corresponds to the 2-point BBDF method lies outside the close region. From the plot, the BBDF method when r = 2 is *A*-stable, r = 1 and r = 5/8 is almost *A*-stable. Hence, the method derived is suitable for solving stiff ODEs

V. IMPLEMENTATION OF 2-POINT BBDF METHOD

In this section, the application of a Newton-type scheme for obtaining the calculation of y_{n+1} , y_{n+2} to some stiff equations are described. The 2-point BBDF method can be written in general form as

$$\left.\begin{aligned} y_{n+1} &= \theta_1 y_{n+2} + \alpha_1 h f_{n+1} + \psi_1 \\ y_{n+2} &= \theta_2 y_{n+1} + \alpha_2 h f_{n+2} + \psi_2 \end{aligned}\right\} \tag{5.1}$$

with ψ_1 and ψ_2 are the backvalues.

Equation (5.1) in matrix-vector form is equivalent to

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

with

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, Y_{n+1,n+2} = \begin{bmatrix} y_{n+1} \\ y_{n+2} \end{bmatrix}, A = \begin{bmatrix} 0 & \theta_1 \\ \theta_2 & 0 \end{bmatrix}, B = \begin{bmatrix} \alpha_1 & 0 \\ 0 & \alpha_2 \end{bmatrix},$$

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

Let

$$\hat{F}_{n+1,n+2} = (I - A) Y_{n+1,n+2} - hBF_{n+1,n+2} - \xi_{n+1,n+2} = 0 \tag{5.2}$$

To approximate this solution, select $Y_{n+1,n+2}^{(i)}$ and generate $Y_{n+1,n+2}^{(i+1)}$ by applying Newton's Iteration to the system (5.2) to obtain

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

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

Choosing the step size

Step size adjustment for 2-Point BBDF is as been stated earlier. On any given step, the user will provide an error tolerance limit, TOL. In the BBDF code, the values of x_{n+1}, x_{n+2} and y_{n+1}, y_{n+2} are accepted if the local truncation error, LTE is less than tolerance limit. The LTE is obtained by taking

$$\text{LTE} = y_{n+2}^{(p+1)} - y_{n+2}^{(p)}$$

where $y_{n+2}^{(p+1)}$ is the (p+1)th order method and $y_{n+2}^{(p)}$ is the pth order method. If the error estimate is greater than the accepted tolerance limit, the value of y_{n+1}, y_{n+2} are rejected, then the step is repeated with halving the current step size. In this case, the step ratio r is 2 . After a successful step, the step size increment is given by

$$h_{new} = c \times h_{old} \times \left(\frac{\text{TOL}}{\text{LTE}} \right)^{\frac{1}{p}} \quad \text{and} \quad \text{if}$$
$$h_{new} > 1.6 \times h_{old} \quad \text{then} \quad h_{new} = 1.6 \times h_{old}$$

where c is the safety factor, p is the order of the method and h_{old} is the step size from previous block. In our case, c is 0.8.

VI. RESULTS

We tested the performance of the 2-point BBDF method on a set of stiff problems. The problems were solved with tolerances $10^{-2}, 10^{-4}$ and 10^{-6} . We will compare the numerical results obtained using 2-point BBDF method with the variable step variable order BDF method which is referred as NBDF. See Suleiman [11] for the details of the algorithm. Below are four of the problems tested.

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

with solution $y(x) = e^{\lambda x} + x$,

Eigenvalues: $\lambda = -20, -30, -100$,

Source: Gear, [4].

Problem 2: $-1000y + 3000 - 2000e^{-x}$, $0 \le x \le 20$, $y(0) = 0$

with solution $3 - 0.998e^{-1000x} - 2.002e^{-x}$.

Problem 3: $\begin{aligned} y_1' &= 998y_1 + 1998y_2 \\ y_2' &= -999y_1 - 1999y_2 \end{aligned}$, $\begin{aligned} y_1(0) &= 1 \\ y_2(0) &= 0 \end{aligned}$, $0 \le x \le 20$

with solution $\begin{aligned} y_1(x) &= 2e^{-x} - e^{-1000x} \\ y_2(x) &= -e^{-x} + e^{-1000x} \end{aligned}$.

Eigenvalues: $\lambda_1 = -1, \lambda_2 = -1000$

Source: Gear, [4].

Problem 4: $\begin{array}{l} y_1' = -1002y_1 + 1000y_2^2 \\ y_2' = y_1 - y_2(1+y_2) \end{array}$, $\begin{array}{l} y_1(0)=1 \\ y_2(0)=1 \end{array}$, $0 \le x \le 20$

with solution $y_1(x) = e^{-2x}, y_2(x) = e^{-x}$

Source: Kaps, [6].

The notations used in the tables take the following meaning:

STPS	:	the total number of steps
TOL	:	the upper bound for the local error estimate
FA	:	the total number of rejected steps (due to convergence failure or local error control)
IST	:	the total number of accepted steps
MAXE	:	maximum error
NBDF	:	implementation of nonblock variable step variable order BDF
BBDF	:	implementation of variable step 2-point BBDF method
TIME	:	the execution time in microseconds

Table 6.1(a): Numerical result for Problem 1 for $\lambda = -30$

TOL	MTD	FA	IST	STPS	MAXE	TIME
10^{-2}	NBDF	7	32	39	4.7188e-02	16075
	BBDF	0	25	25	1.2017e-04	8287
10^{-4}	NBDF	11	53	64	9.0525e-04	25919
	BBDF	0	39	39	2.0600e-06	9275
10^{-6}	NBDF	16	89	105	1.3568e-05	28715
	BBDF	0	74	74	2.5285e-08	11655

Table 6.1(b): Numerical result for Problem 1 for $\lambda = -50$

TOL	MTD	FA	IST	STPS	MAXE	TIME
10^{-2}	NBDF	6	30	36	5.4862e-02	23214
	BBDF	0	26	26	2.3300e-04	8571
10^{-4}	NBDF	10	53	63	6.1625e-04	25435
	BDF	0	39	39	2.8412e-06	9311
10^{-6}	NBDF	14	88	102	7.9504e-06	27589
	BDF	0	75	75	1.9296e-08	11749

Table 6.1(c): Numerical result for Problem 1 for $\lambda = -100$

TOL	MTD	FA	IST	STPS	MAXE	TIME
10^{-2}	NBDF	6	30	36	2.4478e-02	23815
	BBDF	0	26	26	1.7978e-04	8561
10^{-4}	NBDF	11	54	65	5.0758e-04	25834
	BBDF	0	40	40	2.4197e-06	9425
10^{-6}	NBDF	16	88	104	5.0793e-06	28827
	BBDF	0	76	76	2.4604e-08	11863

Table 6.2: Numerical result for Problem 2

TOL	MTD	FA	IST	STPS	MAXE	TIME
10^{-2}	NBDF	5	36	41	5.38298e-03	16643
	BBDF	0	30	30	1.98645e-04	9695
10^{-4}	NBDF	8	74	82	1.97582e-04	21167
	BBDF	0	51	51	2.64614e-06	11168
10^{-6}	NBDF	12	130	142	5.42660e-06	25460
	BBDF	0	109	109	1.00448e-06	15459

Table 6.3: Numerical result for Problem 3

TOL	MTD	FA	IST	STPS	MAXE	TIME
10^{-2}	NBDF	13	58	71	3.5277e-01	17475
	BBDF	0	31	31	2.5644e-04	12567
10^{-4}	NBDF	18	101	119	1.1269e-03	22692
	BBDF	0	53	53	2.5308e-06	16326
10^{-6}	NBDF	22	165	660	6.8001e-06	30318
	BDF	0	122	122	2.9400e-08	24694

Table 6.4: Numerical result for Problem 4

TOL	MTD	FA	IST	STPS	MAXE	TIME
10^{-2}	NBDF	8	48	56	1.3084e-01	23062
	BBDF	0	27	27	1.0739e-04	11547
10^{-4}	NBDF	17	84	101	1.1900e-03	26540
	BBDF	0	47	47	5.4820e-06	14243
10^{-6}	NBDF	20	123	143	6.5959e-06	30981
	BBDF	0	104	104	2.2494e-07	20902

VII. CONCLUSION

For all the problems tested, numerical results shows that the BBDF methods gives better accuracy with reduction of total steps and lesser computational time.

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