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Two–Point Diagonally Implicit Extended Super Class of Block Backward Differentiation Formula for Stiff Initial Value Problems

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Abstract:

In this paper, a diagonal form of the extended super class of block backward differentiation formula is derived. The method is fully implicit and approximates two solution values at a time. By varying a parameter $\rho\epsilon$ (–1,1) in the formula, different sets of formulae can be generated. Analysis of the method indicated that the method is both zero and A–stable, hence, suitable for solving stiff initial value problems. Comparison of the method with some existing algorithms showed its advantage in terms of accuracy over some methods.

Keywords: Initial Value Problems, Stiff, zero stability, A–Stability, diagonally implicit method.

1. Introduction (Times New Roman, bold, 10pts applies to all titles)

Consider the Initial Value Problem (IVP):

$$y' = (x,), \qquad y(a) = y_o, \quad a \le x \le b \qquad (1)$$

where the function $f(x,y)$ is continuous and differentiable on the interval $a \le x \le b$ and is assumed to satisfy the Liptschiptz condition for the existence and uniqueness of solution (Lambert, 1973). Problem (1) can be stiff or non stiff. Stiff IVPs describe differential equations where different physical phenomena acting on different time scales occur simultaneously (Brugnano et al 2011). Dahlquist (1973) described stiff problems as systems containing very fast components as well as very slow components". Such problems are found in mechanics, electrical circuits, vibrations, chemical reactions, kinetics etc. Methods for solving stiff problems of the type (1) can be sequential or block methods. Examples of sequential methods for solving (1) are Curtiss, C. and Hirschfelder (1952), Cash J.R.(1980), Cash J.R.(2000). Block methods for solving the stiff IVP (1) include Ibrahim et al (2007), Musa et al (2012), Suleiman et al (2014), Suleiman et al (2013). There are also diagonally implicit block methods for solving stiff IVPs as found in Abasi et al (2014), Zawawi et al (2012), Musa et al (2016).

This research is motivated by the work of Musa et al (2020). The paper presents the diagonal form of the Extended Two-point Super Class of Block Backward Differentiation Formula (2ESBBDF) of Musa et al (2020) by introducing a lower triangular matrix in the formula in the method.

2. Derivation of the Method

Consider the 2ESBBDF method developed by Musa et al (2020)

$$\sum_{j=0}^{3} \alpha_{j,i} y_{n+j-1} = h\beta_{k,i}(f_{n+k} - \rho f_{n+k-2}), \quad k = i = 1, 2 \qquad (2)$$

where , $k = i = 1$ stands for the first point formula, and $k = i = 2$ stands for the second point formula.

In this research, we proposed the diagonal form the formula 2 to come up with the method:

$$\sum_{j=0}^{1+k} \alpha_{j,i} y_{n+j-1} = h\beta_{k,i}(f_{n+k} - \rho f_{n+k-2}), \quad k = i = 1,2 . \qquad (3)$$

which we shall refer to as Diagonally Implicit Extended Two–point Super Class of Block Backward Differentiation Formula (DIE2SBBDF). $k = i = 1$ represents the first point formula while $k = i = 2$ represents the second point formula.

To derive the first point ($k = i = 1$) of the method (3), define the linear operator L_1 associated with the method DIE2SBBDF by:

$$L_1[y(x_n), \mathrm{h}]: \alpha_{0,1} y(x_n - h) + \alpha_{1,1} y(x_n) + \alpha_{2,1} y(x_n + \mathrm{h}) - h\beta_{1,1}\big(f(x_n + \mathrm{h}) - \rho f(x_n - \mathrm{h})\big) = 0, \qquad (4)$$

and for the second point ($k = i = 2$), by:

$$L_2[y(x_n), \mathrm{h}]: \alpha_{0,2} y(x_n - h) + \alpha_{1,2} y(x_n) + \alpha_{2,2} y(x_n + \mathrm{h}) + \alpha_{3,2} y(x_n + 2\mathrm{h}) - h\beta_{2,2}\big(f(x_n + 2\mathrm{h}) - \rho f(x_n)\big) = 0. \qquad (5)$$

To obtain the first point, we expand (4) as Taylor's series about x_n and collect like terms to obtain:

$$C_{0,1} y(x_n) + C_{1,1} h y'(x_n) + C_{2,1} h^2 y''(x_n) + \cdots = 0. \qquad (6)$$

where

$$\left.\begin{aligned} C_{0,1} &= \alpha_{0,1} + \alpha_{1,1} + \alpha_{2,1} = 0 \\ C_{1,1} &= -\alpha_{0,1} + \alpha_{2,1} + \beta_{1,1}(\rho - 1) = 0 \\ C_{2,1} &= \tfrac{1}{2}\alpha_{0,1} + \tfrac{1}{2}\alpha_{2,1} - \beta_{1,1}(\rho + 1) = 0 \end{aligned}\right\} \qquad (7)$$

The coefficient of the first point $(\alpha_{2,1})$, is normalized to 1. Solving equation (7) simultaneously gives the values of $\alpha_{j,1}'s$ and $\beta_{j,1}'s$ as:

$\alpha_{0,1} = \frac{3\rho+1}{\rho+3}$, $\alpha_{1,1} = -\frac{4(\rho+1)}{\rho+3}$, $\alpha_{2,1} = 1$, and $\beta_{1,1} = \frac{2}{\rho+3}$

Substituting these values into (4), the first point is obtained as:

$$y_{n+1} = \frac{3\rho+1}{\rho+3} y_{n-1} + \frac{4(\rho+1)}{\rho+3} y_n + \frac{2h}{\rho+3} f_{n+1} - \frac{2h\rho}{\rho+3} f_{n-1} \qquad (8)$$

Using (5) and adopting a similar procedure, the second point is obtained as:

$$y_{n+2} = -\frac{2(\rho-1)}{\rho+11} y_{n-1} - \frac{3(\rho+3)}{\rho+11} y_n + \frac{6(\rho+3)}{\rho+11} y_{n+1} + \frac{6h}{\rho+11} f_{n+2} - \frac{6h\rho}{\rho+11} f_n \qquad (9)$$

Thus, the DIE2SBBDF method is therefore given by:

$$\left.\begin{aligned} y_{n+1} &= \frac{3\rho+1}{\rho+3} y_{n-1} + \frac{4(\rho+1)}{\rho+3} y_n + \frac{2h}{\rho+3} f_{n+1} - \frac{2h\rho}{\rho+3} f_{n-1} \\ y_{n+2} &= -\frac{2(\rho-1)}{\rho+11} y_{n-1} - \frac{3(\rho+3)}{\rho+11} y_n + \frac{6(\rho+3)}{\rho+11} y_{n+1} + \frac{6h}{\rho+11} f_{n+2} - \frac{6h\rho}{\rho+11} f_n \end{aligned}\right\} \qquad (10)$$

For the purpose of maintaining absolute stability of the method, Suleiman et al (2014) justified the use of ρ in the interval $(-1,1)$ for the super class block backward differentiation formulae. In this paper, the value $\rho = -\frac{1}{2}$ is chosen to illustrate the performance of the method, which gave rise to the formula:

$$\left.\begin{aligned} y_{n+1} &= \tfrac{1}{5} y_{n-1} + \tfrac{4}{5} y_n + \tfrac{4}{5} h f_{n+1} + \tfrac{2}{5} h f_{n-1} \\ y_{n+2} &= \tfrac{2}{7} y_{n-1} - \tfrac{5}{7} y_n + \tfrac{10}{7} y_{n+1} + \tfrac{4}{7} h f_{n+2} + \tfrac{2}{7} h f_n \end{aligned}\right\} \qquad (11)$$

Any value of $\rho \in (-1,1)$ gives a different set of the DIE2SBBDF which can be analyzed and implemented for the solution of stiff IVPs. The method is of order 3.

3. Stability analysis of the method

Apply the test differential equation:

$$y' = \lambda y, \qquad \lambda < 0, \qquad (12)$$

into equation (11) to obtain:

$$\left.\begin{aligned} y_{n+1} &= \tfrac{1}{5} y_{n-1} + \tfrac{4}{5} y_n + \tfrac{4}{5}\lambda h y_{n+1} + \tfrac{2}{5}\lambda h y_{n-1} \\ y_{n+2} &= \tfrac{2}{7} y_{n-1} - \tfrac{5}{7} y_n + \tfrac{10}{7} y_{n+1} + \tfrac{4}{7}\lambda h y_{n+2} + \tfrac{2}{7}\lambda h y_n \end{aligned}\right\} \qquad (13)$$

Let $\lambda h = \bar{h}$ and rewrite (13) in matrix form to obtain:

$$\begin{pmatrix} 1 - \frac{4}{5}\bar{h} & 0 \\ -\frac{10}{7} & 1 - \frac{4}{7}\bar{h} \end{pmatrix} \begin{pmatrix} y_{n+1} \\ y_{n+2} \end{pmatrix} = \begin{pmatrix} \frac{1}{5} + \frac{2}{5}\bar{h} & \frac{4}{5} \\ \frac{2}{7} & -\frac{5}{7} + \frac{2}{7}\bar{h} \end{pmatrix} \begin{pmatrix} y_{n-1} \\ y_n \end{pmatrix} \qquad (14)$$

Let $A = \begin{pmatrix} 1 - \frac{4}{5}\bar{h} & 0 \\ -\frac{10}{7} & 1 - \frac{4}{7}\bar{h} \end{pmatrix}$ and $B = \begin{pmatrix} \frac{1}{5} + \frac{2}{5}\bar{h} & \frac{4}{5} \\ \frac{2}{7} & -\frac{5}{7} + \frac{2}{7}\bar{h} \end{pmatrix}$.

To obtain the stability polynomial of the method (11), we evaluate the determinant of $(At - B = 0)$ to get:

$$R(t, \bar{h}) = t^2 - \frac{43}{35} t^2 \bar{h} - \frac{22}{35} t - \frac{8}{7} t\bar{h} + \frac{16}{35} t^2 \bar{h}^2 + \frac{16}{35} t\bar{h}^2 - \frac{13}{35} - \frac{8}{35}\bar{h} + \frac{4}{35}\bar{h}^2 = 0 \qquad (15)$$

Substitute $\bar{h} = 0$ into equation (15) gives the first characteristics polynomial as:

$$t^2 - \frac{22}{35} t - \frac{13}{35} = 0 \qquad (16)$$

Solving for t in equation (16) gives:

$|t_1| = 1$, $|t_2| = \frac{13}{35}$

By these values of t, the method (11) is zero stable.

The stability region of the method (11) is determined by substituting $t = e^{i\theta}$ into (15). The graph of stability region for the method is plotted using Maple software and presented as follows:

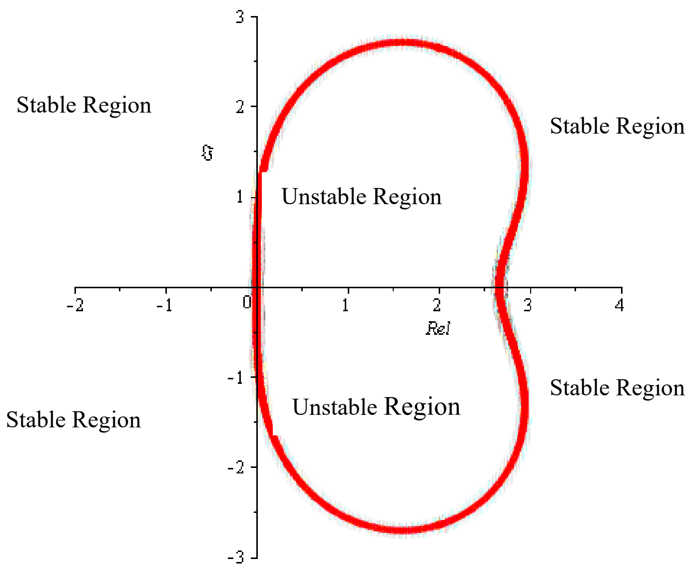

Figure 1: Stability Region of the 2-point DIE2SBBDF when $\rho=-\frac{1}{2}$.

From Figure 1, the stability region of the method covers the entire negative half plane. Hence, the method is A–Stable and is suitable for solving stiff IVPs.

4. Implementation of the method

The method is implemented via Newton's iteration. We begin by defining the error of the method. Let y_i and $y(x_i)$ be respectively, the approximate and exact solution of y_{n+1} and y_{n+2}. Then the absolute error is given by:

$$(error_i)_t = |(y_i)_t - y(x_i)_t|. \quad (17)$$

The maximum error is given by:

$$\text{MAXE}=\max_{1\le i\le T}\left(\max_{1\le i\le N}(error_i)_t\right) \quad (18)$$

Where T is the total number of steps and N is the number of equations.

From (11), Let

$$\left.\begin{aligned} F_1 &= y_{n+1} - \frac{4}{5}hf_{n+1} - \frac{2}{5}hf_{n-1} - \varepsilon_1 \\ F_2 &= y_{n+2} - \frac{10}{7}y_{n+1} - \frac{4}{7}hf_{n+2} - \frac{2}{7}hf_n - \varepsilon_2 \end{aligned}\right\} \quad (19)$$

where $\varepsilon_1 = \frac{1}{5}y_{n-1} + \frac{4}{5}y_n$ and $\varepsilon_2 = \frac{2}{7}y_{n-1} - \frac{5}{7}y_n$ denote the back values.

Let $y_{n+1}^{(i+1)}$ denotes the $(i+1)^{th}$ iteration and

$$e_{n+j}^{(i+1)} = y_{n+j}^{(i+1)} - y_{n+j}^{(i)}, \qquad j = 1,2. \quad (20)$$

The Newton's iteration for the DIE2SBBDF method when $\rho = -\frac{1}{2}$ takes the form

$$e_{n+j}^{(i+1)} = -\left[F_j(y_{n+j}^{(i)})\right]^{-1} F_j(y_{n+j}^{(i)})], \qquad j = 1,2. \quad (21)$$

Equation (21) can be rewritten as:

$$[F'_j(y_{n+j,n+2}^{(i)})]e_{n+j}^{(i+1)} = -\left[F_j(y_{n+j}^{(i)})\right], \qquad j = 1,2. \quad (22)$$

Or

$$[F_j'(y_{n+j,n+2}^{(i)})]e_{n+1,n+2}^{(i+1)} = -[F_j(y_{n+j,n+2}^{(i)})], \quad (23)$$

The matrix form of equation (23) is written as:

$$\begin{pmatrix} 1-\frac{4h\partial f_{n+1}}{5\partial y_{n+1}} & 0 \\ -\frac{10}{7} & 1-\frac{4h\partial f_{n+2}}{7\partial y_{n+2}} \end{pmatrix}\begin{pmatrix} e_{n+1}^{(n+1)} \\ e_{n+2}^{(i+1)}\end{pmatrix} = \begin{pmatrix} -1 & 0 \\ \frac{10}{7} & -1\end{pmatrix}\begin{pmatrix} y_{n+1}^{(i)} \\ y_{n+2}^{(i)}\end{pmatrix} + h\begin{pmatrix}\frac{2}{5} & 0\\ 0 & \frac{2}{7}\end{pmatrix}\begin{pmatrix} f_{n-1}^{(i)} \\ f_n^{(i)}\end{pmatrix} + h\begin{pmatrix}\frac{4}{5}&0\\0&\frac{4}{7}\end{pmatrix}\begin{pmatrix}f_{n+1}^{(i)}\\f_{n+2}^{(i)}\end{pmatrix}+\begin{pmatrix}\varepsilon_1\\ \varepsilon_2\end{pmatrix} \quad (24)$$

5. Numerical Results

To test the performance of the method, the following problems are considered:

Problem 1: (Ibrahim *et al*, 2007)

$$y' = -100\sin(x-y), \quad y(0) = 0, \qquad x \in [0,3]$$

Exact solution: $y(x) = \frac{\sin x - 0.01\cos x + 0.01e^{-100x}}{1.0001}$

Problem 2: (Ibrahim *et al,* 2007)

$$y_1' = 198y_1 + 199y_2, \qquad y_1(0) = 1$$
$$y_2' = 398y_1 - 399y_2, \qquad y_2(0) = -1$$

$x \in [0,10]$

Exact solution:

$$y_1(x) = e^{-x}$$
$$y_2(x) = -e^{-x}$$

Eigenvalues –1 and –200

Problem 3: (Zawawi *et al*, 2012)

$$y_1' = 9y_1 + 24y_2 + 5\cos x - \frac{1}{3}\sin x, \qquad y_1(0) = \frac{4}{3}$$
$$y_2' = -24y_1 - 51y_2 - 9\cos x - \frac{1}{3}\sin x, \qquad y_2(0) = \frac{2}{3}$$

$x \in [0,2]$

Exact solution:

$$y_1(x) = 2e^{-3x} - e^{-39x} + \frac{1}{3}\cos x$$
$$y_2(x) = -e^{-3x} + 2e^{-39x} - \frac{1}{3}\cos x$$

Eigen values: –3 and –39

The following are tables of results indicating the maximum error and the total steps taken to solve each of the problems. The results are compared with some known successful block backward differentiation formula based algorithms. The notations used in the tables are:

h = Step size.

NS = Total number of steps.

MAXE = Maximum error.

Time = Computation time in seconds.

2BBDF = 2 point Block Backward Differentiation Formula. Ibrahim *et al* (2007)

2ESBBDF = Two–point Extended Super Class of Block Backward Differentiation Formula. Musa and Zainab (2020)

DIE2SBBDF=Diagonally Implicit Extended 2–point Super Class of Block Backward Differentiation Formula

Table 1: **Numerical Result for problem 1 when $\rho = -\frac{1}{2}$**

h	Method	NS	MAXE	Time
10^{-2}	2ESBBDF	500	1.83217e-004	0.32440
	2BBDF	500	7.32490e-004	0.18360
	DIE2SBBDF	500	1.83082e-004	0.01899

10^{-3}	2ESBBDF 2BBDF DIE2SBBDF	5000 5000 5000	8.05338e-005 5.67110e-004 1.03200e-004	0.01989 0.22660 0.01962
10^{-4}	2ESBBDF 2BBDF DIE2SBBDF	50,000 50,000 50,000	1.26692e-006 7.18301e-005 1.35868e-006	0.08274 1.13400 0.04326
10^{-5}	2ESBBDF 2BBDF DIE2SBBDF	500,000 500,000 500,000	1.32740e-008 7.33991e-006 1.39582e-008	0.33680 1.24700 0.25680
10^{-6}	2ESBBDF 2BBDF DIE2SBBDF	5.000,000 5,000,000 5,000,000	1.33363e-010 7.35563e-007 1.39958e-010	2.38100 3.07600 2.36400

Table 2: Numerical Result for problem 2 when $\rho = -\frac{1}{2}$

h	Method	NS	MAXE	Time
10^{-2}	2ESBBDF 2BBDF DIE2SBBDF	500 500 500	1.26692e-004 7.18323e−003 1.35868e-004	0.018825 0.15740 0.016963
10^{-3}	2ESBBDF 2BBDF DIE2SBBDF	5000 5000 5000	1.32740e-006 7.34012e-004 1.39582e-006	0.02873 0.55790 0.02798
10^{-4}	2ESBBDF 2BBDF DIE2SBBDF	50,000 50,000 50,000	1.33363e-008 7.35584e-005 1.39958e-008	0.15610 0.97790 0.14230
10^{-5}	2ESBBDF 2BBDF DIE2SBBDF	500,000 500,000 500,000	1.33425e-010 7.35741e-006 1.39996e-010	1.43900 1.61700 1.31200
10^{-6}	2ESBBDF 2BBDF DIE2SBBDF	5.000,000 5,000,000 5,000,000	5.07977e-012 7.35742e-007 1.13680e-011	12.50000 8.17400 12.27000

Table 3: Numerical Result for problem 3 when $\rho = -\frac{1}{2}$

h	Method	NS	MAXE	Time
10^{-2}	2ESBBDF 2BBDF DIE2SBBDF	500 500 500	7.10662e-002 1.24297e-001 1.17385e-001	0.04397 0.17950 0.02165
10^{-3}	2ESBBDF 2BBDF DIE2SBBDF	5000 5000 5000	3.31095e-003 5.17278e-002 3.77465e-003	0.06397 0.29190 0.06353
10^{-4}	2ESBBDF 2BBDF DIE2SBBDF	50,000 50,000 50,000	3.96606e-005 5.64465e-00 34.19726e-005	0.49060 1.15100 0.49070
10^{-5}	2ESBBDF 2BBDF DIE2SBBDF	500,000 500,000 500,000	4.03921e-007 5.69228e-004 4.24170e-007	4.74900 1.48300 4.71600
10^{-6}	2ESBBDF 2BBDF DIE2SBBDF	5.000,000 5,000,000 5,000,000	4.04661e-009 5.69705e-005 4.24617e-009	47.26000 4.89500 47.07000

From Tables 1–3, the accuracy of the DIE2SBBDF is clearly seen when the maximum error (MAXE) of the method is compared with that of the other two algorithms. For all the problems tested, the method is seen to have outperformed the 2BBDF method in terms of accuracy. However, the method competes with the 2ESBBDF in terms of accuracy and performed better in computation time when compared with the 2ESBBDF.

To give a visualization of performance of the methods presented in the Tables 1–3, a graph of $Log_{10}(MAXE)$ against h is plotted and presented in Figure 2–4.

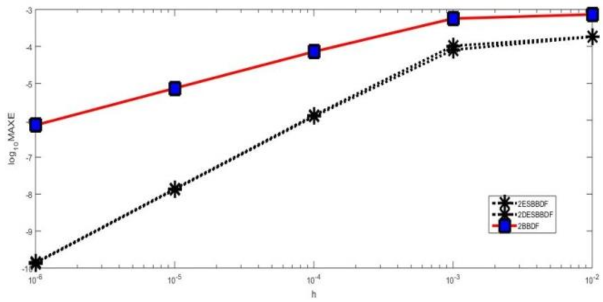

Figure 2: Graph of $Log_{10}(MAXE)$against h for problem 1 when $\rho = -\frac{1}{2}$

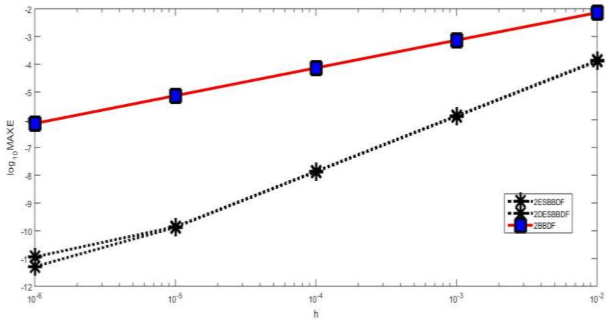

Figure 3: Graph of $Log_{10}\ (MAXE)$ against h for problem 2 when $\rho = -\frac{1}{2}$

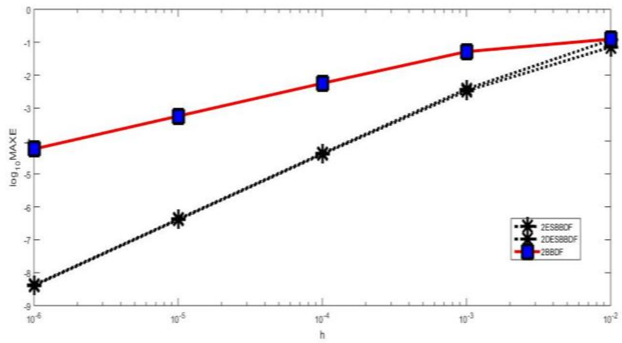

Figure 4: Graph of $Log_{10}\ (MAXE)$ against h for problem 3 when $\rho = -\frac{1}{2}$

Again, the graphs also show that the scaled errors of the DIE2SBBDF method are smaller when compared with that of the 2BBDF method. It can also be seen that the DIE2SBBDF competes with the 2ESBBDF as most of the points coincided.

6. Conclusion

A method of order 3 of the type, super class of block backward differentiation formula, which is suitable for solving stiff initial value problems, is developed. The stability analysis has shown that the method is both zero and A–stable. Accuracy and the execution time of the derived method are compared with the existing 2–point extended super class of block backward differentiation. The comparison shows that the new method outperformed the existing two point block backward differentiation formula in terms of accuracy. The computation time for the new method is seen to be competitive. The graphs also have shown that the scaled errors of the extended two point super class of block backward differentiation formula are smaller when compared with that of the two point block backward differentiation formula.

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