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A New Fifth Order Implicit Block Method for Solving First Order Stiff Ordinary Differential Equations

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ABSTRACT

A new implicit block backward differentiation formula that computes 3–points simultaneously is derived. The method is of order 5 and solves system of stiff ordinary differential equations (ODEs). The stability analysis indicates that the method is A–stable. Numerical results show that the method outperformed some existing block and non-block methods for solving stiff ODEs.

Keywords: A-Stability, implicit block method, order of a block method, stiff, ordinary differential equations.

1. INTRODUCTION

In the cause of modeling various physical problems arising in science and engineering, a special class of ordinary differential equations (ODEs) known as stiff arise. It has the form given by:

$$y' = f(x, y) \qquad y(a) = y_0 \qquad x \in [a, b] \tag{1}$$

A system of stiff ODEs may contain in its solution, components with slow and rapidly decay rates and this behaviour makes it difficult to solve stiff problems using explicit numerical methods. There is therefore an increasing demand in developing implicit numerical methods for such problems. Many numerical methods have been developed to solve (1) sequentially in Curtiss *et al.* (1952), Gear (1971), Cash (1980), Hairer *et al.* (1993), Lambert (1973), Roser (1967) and Bohmer *et al*. (1984).

There are other classes of methods suggested by Hall et al (1976) that computes a block of approximations simultaneously e.g. Fatunla (1991), Watanabe (1978), Majid et al (2007), Ibrahim et al (2007), Shampine et al (1969), Voss *et al.* (1997), Andria *et al.* (1973), Musa *et al*. (2011), *Musa et al.* (2012) and Suleiman *et al.* (2013).

Consider the fixed step 3–point block backward differentiation formula (BBDF) :

$$\sum_{j=0}^{5} \alpha_{j,i} y_{n+j-2} = h\beta_{k,i} f_{n+k} \qquad k=i=1,2,3. \tag{2}$$

developed in Ibrahim *et al.* (2007) for the solution of (1).

The formula (2) has the coefficient $\beta_{k-1,i}=0$ and is found to be efficient for solving stiff ODEs. The focus of this paper is to develop a new implicit block method of the form (2), but with the coefficient $\beta_{k-1,i} \neq 0$; that will compute 3 solution values simultaneously. The aim is to develop a more accurate scheme that will solve (1) without altering with the order of (2). Strategies for improving accuracy, order and efficiency of multistep methods have been suggested by Hairer *et al*. (1993) and include adding future point, off-step point and using higher derivatives. Our method will have the form:

$$\sum_{j=0}^{5} \alpha_{j,i} y_{n+j-2} = h\beta_{k,i} \left(f_{n+k} - \rho f_{n+k-1} \right) \qquad k=i=1,2,3. \tag{3}$$

where ρ is a free parameter to be chosen from the interval $(-1,1)$ and $\beta_{k-1,i} = \rho\beta_{k,i}$. This paper uses the value $\rho = \frac{1}{2}$ and has found an A–stable method.

The remaining sections of the paper will present the derivation of the method and its order, the stability analysis, the implementation of the method, test problems used and numerical results. Finally, a conclusion is given.

2. DERIVATION

This section describes the derivation of the fixed step 3–point block method. Given 3 back values x_{n-2}, x_{n-1} and x_n, we shall develop a formula that will compute 3 solution values; namely y_{n+1}, y_{n+2} and y_{n+3} at the points x_{n+1}, x_{n+2} and x_{n+3} respectively. The procedure will involve Taylor series expansion of the linear operator

$$\begin{aligned} L_i\left[y(x_n),h\right] = {} & \alpha_{0,i}y(x_n-2h)+\alpha_{1,i}y(x_n-h)+\alpha_{2,i}y(x_n)+\alpha_{3,i}y(x_n+h) \\ & +\alpha_{4,i}y(x_n+2h)+\alpha_{5,i}y(x_n+3h) \\ & -h\beta_{k,i}\left(f\left(x_n+kh\right)-\rho f\left(x_n+(k-1)h\right)\right)=0 \end{aligned} \tag{4}$$

where $k=i=1,2,3.$

When $k=i=1$, the formula obtained corresponds to the first point, $k=i=2$ corresponds to the second point and $k=i=3$ corresponds to the third point. Expanding (4) using Taylor's series gives a set of equations to be solved simultaneously. For the first point, the coefficient $\alpha_{3,1}$ is normalized to 1; for the second point, $\alpha_{4,2}$ is normalized and for the third point, $\alpha_{5,3}$ is normalized. Substituting $\rho=\frac{1}{2}$, the following implicit 3–point block formula is obtained:

$$
\begin{aligned}
y_{n+1} &= -\frac{7}{20}y_{n-2} + 3y_{n-1} - 5y_n + \frac{15}{4}y_{n+2} - \frac{2}{5}y_{n+3} + 3hf_n - 6hf_{n+1} \\
y_{n+2} &= -\frac{2}{25}y_{n-2} + \frac{11}{20}y_{n-1} - \frac{9}{5}y_n + \frac{13}{5}y_{n+1} - \frac{27}{100}y_{n+3} - \frac{3}{5}hf_{n+1} \\
&\quad + \frac{6}{5}hf_{n+2} \\
y_{n+3} &= \frac{27}{262}y_{n-2} - \frac{85}{131}y_{n-1} + \frac{230}{131}y_n - \frac{360}{131}y_{n+1} + \frac{665}{262}y_{n+2} - \frac{30}{131}hf_{n+2} \\
&\quad + \frac{60}{131}hf_{n+3}
\end{aligned}
\tag{5}
$$

The error constant for the formula (5) is:

$$
C_6 = \begin{pmatrix} \frac{3}{20} \\ \frac{1}{20} \\ -\frac{11}{131} \end{pmatrix}.
$$

indicating that the method is of order 5.

3. STABILITY ANALYSIS

This section presents the stability analysis of the method (5). The method developed will be examined by applying the test differential equation:

$$
y' = \lambda y \tag{6}
$$

where λ is complex constant with $\mathrm{Re}(\lambda) < 0.$

Rewriting the formula (5) in matrix form gives:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \end{pmatrix} = \begin{pmatrix} -\frac{7}{20} & 3 & -5 \\ -\frac{2}{25} & \frac{11}{20} & -\frac{9}{5} \\ \frac{27}{262} & \frac{-85}{131} & \frac{230}{131} \end{pmatrix}\begin{pmatrix} y_{n-2} \\ y_{n-1} \\ y_{n} \end{pmatrix} + \begin{pmatrix} 0 & \frac{15}{4} & -\frac{2}{5} \\ \frac{13}{5} & 0 & -\frac{27}{100} \\ -\frac{360}{131} & \frac{665}{262} & 0 \end{pmatrix}\begin{pmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \end{pmatrix}$$

$$+h\begin{pmatrix} 0 & 0 & 3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} f_{n-2} \\ f_{n-1} \\ f_{n} \end{pmatrix} + h\begin{pmatrix} -6 & 0 & 0 \\ -\frac{3}{5} & \frac{6}{5} & 0 \\ 0 & -\frac{30}{131} & \frac{60}{131} \end{pmatrix}\begin{pmatrix} f_{n+1} \\ f_{n+2} \\ f_{n+3} \end{pmatrix} \tag{7}$$

and equation (7) is equivalent to:

$$\begin{pmatrix} 1 & -\frac{15}{4} & \frac{2}{5} \\ -\frac{13}{5} & 1 & \frac{27}{100} \\ \frac{360}{131} & -\frac{665}{262} & 1 \end{pmatrix}\begin{pmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \end{pmatrix} = \begin{pmatrix} -\frac{7}{20} & 3 & -5 \\ -\frac{2}{25} & \frac{11}{20} & -\frac{9}{5} \\ \frac{27}{262} & \frac{-85}{131} & \frac{230}{131} \end{pmatrix}\begin{pmatrix} y_{n-2} \\ y_{n-1} \\ y_{n} \end{pmatrix} + h\begin{pmatrix} 0 & 0 & 3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} f_{n-2} \\ f_{n-1} \\ f_{n} \end{pmatrix}$$

$$+h\begin{pmatrix} -6 & 0 & 0 \\ -\frac{3}{5} & \frac{6}{5} & 0 \\ 0 & -\frac{30}{131} & \frac{60}{131} \end{pmatrix}\begin{pmatrix} f_{n+1} \\ f_{n+2} \\ f_{n+3} \end{pmatrix} \tag{8}$$

Equation (8) can be represented in the following form:

$$A_0 Y_m = A_1 Y_{m-1} + h\left(B_0 F_{m-1} + B_1 F_m\right) \tag{9}$$

where

$$A_0 = \begin{pmatrix} 1 & -\frac{15}{4} & \frac{2}{5} \\ -\frac{13}{5} & 1 & \frac{27}{100} \\ \frac{360}{131} & -\frac{665}{262} & 1 \end{pmatrix}, \qquad Y_m = \begin{pmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \end{pmatrix},$$

$$A_1 = \begin{pmatrix} -\frac{7}{20} & 3 & -5 \\ -\frac{2}{25} & \frac{11}{20} & -\frac{9}{5} \\ \frac{27}{262} & \frac{-85}{131} & \frac{230}{131} \end{pmatrix}, \qquad Y_{m-1} = \begin{pmatrix} y_{n-2} \\ y_{n-1} \\ y_n \end{pmatrix},$$

$$B_0 = \begin{pmatrix} 0 & 0 & 3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad F_{m-1} = \begin{pmatrix} f_{n-2} \\ f_{n-1} \\ f_n \end{pmatrix},$$

$$B_1 = \begin{pmatrix} -6 & 0 & 0 \\ -\frac{3}{5} & \frac{6}{5} & 0 \\ 0 & -\frac{30}{131} & \frac{60}{131} \end{pmatrix}, \qquad F_{m+1} = \begin{pmatrix} f_{n+1} \\ f_{n+2} \\ f_{n+3} \end{pmatrix}.$$

Applying (6) into (9) and letting $\overline{h} = \lambda h$, we have:

$$\left(A_0 - \overline{h}B_1\right)Y_m = \left(A_1 + \overline{h}B_0\right) = 0 \tag{10}$$

To find the stability polynomial, the following equation is evaluated:

$$\det\left(t\left(A_0 - \overline{h}B_1\right) - \left(A_1 + \overline{h}B_0\right)\right) = 0 \tag{11}$$

to obtain the stability polynomial:

$$
\begin{aligned}
R(t,\bar{h}) = {} & \frac{53}{1310} + \frac{15\bar{h}}{1048} - \frac{7881t}{5240} - \frac{4077\bar{h}t}{2620} - \frac{558\bar{h}^{2}t}{665} + \frac{14109t^{2}}{1310} \\
& + \frac{50373\bar{h}t^{2}}{5240} + \frac{10737\bar{h}^{2}t^{2}}{1310} - \frac{54\bar{h}^{3}t^{2}}{131} - \frac{48767t^{3}}{5240} + \frac{20409\bar{h}t^{3}}{1310} \\
& - \frac{7038\bar{h}^{2}t^{3}}{655} + \frac{432\bar{h}^{3}t^{3}}{131} = 0
\end{aligned} \tag{12}
$$

To show that the method is zero stable, we set $\bar{h} = 0$ in (12) to obtain the following first characteristic polynomial:

$$
\frac{53}{1310} - \frac{7881t}{5240} + \frac{14109t^{2}}{1310} - \frac{48767t^{3}}{5240} = 0 \tag{13}
$$

Solving equation (13) for t, we have:

t=1, t=0.0357884, t=0.12147

Thus by the definition of zero stability, the method (5) is zero stable. The plot of the stability region is given below and it shows that the method is A – stable.

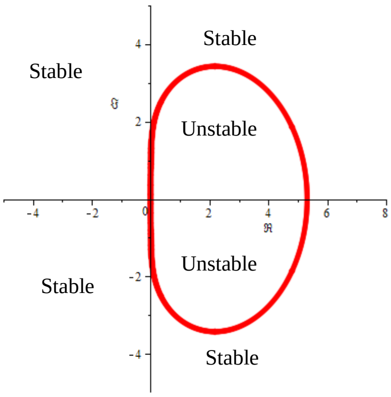

Figure 1: Stability region of the 3-point when $\rho = \frac{1}{2}$.

4. IMPLEMENTATION OF THE METHOD

Newton's iteration is employed to implement the method. We consider the implementation when $\rho = \frac{1}{2}$ and the same applies for any value of $\left(-1,1\right)$. The iteration is described below.

Let y_i and $y(x_i)$ be the approximate and exact solutions of (1) respectively. The absolute error is defined by

$$\left(error_i\right)_t = \left|(y_i)_t - (y(x_i))_t\right| \tag{14}$$

The maximum error is given by:

$$MAXE = \max_{1\le i\le T}\left(\max_{1\le i\le N}\left(error_i\right)_t\right) \tag{15}$$

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

Let $y_{n+1}^{(i+1)}$ denote the $(i+1)^{th}$ iterate and

$$e_{n+j}^{(i+1)} = y_{n+j}^{(i+j)} - y_{n+j}^{(i)} \qquad j = 1, 2, 3. \tag{16}$$

Let

$$\begin{aligned}
F_1 &= y_{n+1} - \frac{15}{4}y_{n+2} + \frac{2}{5}y_{n+3} - 3hf_n + 6hf_{n+1} - \xi_1 \\
F_2 &= y_{n+2} - \frac{13}{5}y_{n+1} + \frac{27}{100}y_{n+3} + \frac{3}{5}hf_{n+1} - \frac{6}{5}hf_{n+2} - \xi_2 \\
F_3 &= y_{n+3} + \frac{360}{131}y_{n+1} - \frac{665}{262}y_{n+2} + \frac{30}{131}hf_{n+2} - \frac{60}{131}hf_{n+3} - \xi_3
\end{aligned} \tag{17}$$

where

$$\begin{aligned}
\xi_1 &= \left(-\frac{7}{20} y_{n-2} + 3y_{n-1} - 5y_n \right) \\
\xi_2 &= \left(-\frac{2}{25} y_{n-2} + \frac{11}{20} y_{n-1} - \frac{9}{5} y_n \right) \\
\xi_3 &= \left(\frac{27}{262} y_{n-2} - \frac{85}{131} y_{n-1} + \frac{230}{131} y_n \right)
\end{aligned} \tag{18}$$

Then the iteration takes the form:

$$y_{n+j}^{(i+1)} = y_{n+j}^{(i)} - \left[F_j\left(y_{n+j}^{(i)}\right) \right] \left[F_j^{'}\left(y_{n+j}^{(i)}\right) \right]^{-1}, \quad j = 1,2,3. \tag{19}$$

which can be written as

$$\left[F_j^{'}\left(y_{n+j}^{(i)}\right) \right] e_{n+j}^{(i+1)} = -\left[F_j\left(y_{n+j}^{(i)}\right) \right], \quad j = 1,2,3. \tag{20}$$

Equation (20) is equivalent to the following matrix form:

$$J \begin{pmatrix} e_{n+1}^{(i+1)} \\ e_{n+2}^{(i+1)} \\ e_{n+3}^{(i+1)} \end{pmatrix} = B \begin{pmatrix} y_{n+1}^{(i)} \\ y_{n+2}^{(i)} \\ y_{n+3}^{(i)} \end{pmatrix} + Ch \begin{pmatrix} f_{n-2}^{(i)} \\ f_{n-1}^{(i)} \\ f_{n}^{(i)} \end{pmatrix} + Dh \begin{pmatrix} f_{n+1}^{(i)} \\ f_{n+2}^{(i)} \\ f_{n+3}^{(i)} \end{pmatrix} + E \tag{21}$$

where

$$J = \begin{pmatrix} 1 + 6h \dfrac{\delta f_{n+1}}{\delta y_{n+1}} & -\dfrac{15}{4} & \dfrac{2}{5} \\ -\dfrac{13}{5} + \dfrac{3}{5} h \dfrac{\delta f_{n+1}}{\delta y_{n+1}} & 1 - \dfrac{6}{5} h \dfrac{\delta f_{n+2}}{\delta y_{n+2}} & \dfrac{27}{100} \\ \dfrac{360}{131} & -\dfrac{665}{262} + \dfrac{30}{131} h \dfrac{\delta f_{n+2}}{\delta y_{n+2}} & 1 - \dfrac{60}{131} h \dfrac{\delta f_{n+3}}{\delta y_{n+3}} \end{pmatrix},$$

$$B=\begin{pmatrix} -1 & \frac{15}{4} & -\frac{2}{5} \\ \frac{13}{5} & -1 & -\frac{27}{100} \\ -\frac{360}{131} & \frac{665}{262} & -1 \end{pmatrix}, \quad C=\begin{pmatrix} 0 & 0 & 3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$D=\begin{pmatrix} -6 & 0 & 0 \\ -\frac{3}{5} & \frac{6}{5} & 0 \\ 0 & -\frac{30}{131} & \frac{60}{131} \end{pmatrix}, \qquad E=\begin{pmatrix} \xi_1 \\ \xi_2 \\ \xi_3 \end{pmatrix}.$$

Equation (21) is solved for $e^{(i+1)}_{(n+1),(n+2),(n+3)}$.

5. TEST PROBLEMS

The following problems are used to test the performance of the method developed.

Example (1)

$$y' = 5e^{5x}\left(y-x\right)^2 + 1, \quad y(0) = -1, \quad 0 \le x \le 1$$

Exact solution

$y(x) = x - e^{-5x}$

Source: Lee *et al.* (2002).

Example (2)

$$\begin{matrix} y_1' = -20y_1 - 19y_2 \\ y_2' = -19y_1 - 20y_2 \end{matrix}, \quad \begin{matrix} y_1(0) = 2 \\ y_2(0) = 0 \end{matrix}, \quad 0 \le x \le 20$$

Exact solution

$y_1(x) = e^{-39x} + e^{-x}$

$y_2(x) = e^{-39x} - e^{-x}$

Source: Cheney *et al.* (2012).

Example (3)

$$\begin{array}{ll} y_1' = 198y_1 + 199y_2 & y_1(0) = 1 \\ y_2' = -398y_1 - 399y_2 & y_2(0) = -1 \end{array}, \quad 0 \le x \le 10$$

Exact solution

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

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

Eigen values: -1 and -200

Source: Ibrahim *et al.* (2007).

6. NUMERICAL RESULTS

The problems given in the previous section are solved using the method developed, the 1–point non-block BDF and the 3–point BBDF with different step sizes h. The maximum error and the computation time for each problem are given in the tables below.

The following notations are used in the Tables.

h = Step size;
1BDF = 1–point BDF method;
3BBDF = 3–point BBDF method;
3NBBDF = 3–point fifth order new BBDF method;
NS = Total number of integration steps;
MAXE = Maximum Error;
Time = Computation time.

TABLE 1: Numerical results for problem (1)

h	Method	NS	MAXE	Time
10^{-2}	1BDF	100	1.16701e-002	3.25750e-004
	3BBDF	33	2.80735e-002	2.76333e-004
	3NBBDF	33	3.51456e-003	5.52416e-004
10^{-3}	1BDF	1,000	1.24337e-003	1.86442e-003
	3BBDF	333	3.71852e-003	1.81850e-003
	3NBBDF	333	4.90191e-005	4.50367e-003
10^{-4}	1BDF	10,000	1.24935e-004	1.71149e-002
	3BBDF	3,333	3.74700e-004	1.71443e-002
	3NBBDF	3,333	5.20417e-007	4.36918e-002
10^{-5}	1BDF	100,000	1.24994e-005	1.68071e-001
	3BBDF	33,333	3.74970e-005	1.70042e-001
	3NBBDF	33,333	5.25030e-009	4.34808e-001
10^{-6}	1BDF	1,000,000	1.25000e-006	1.68182e+000
	3BBDF	333,333	3.74997e-006	1.70308e+000
	3NBBDF	333,333	5.25648e-011	4.35791e+000

TABLE 2: Numerical results for problem (2)

H	Method	NS	MAXE	Time
10^{-2}	1BDF	2000	6.85453e-002	7.22775e-003
	3BBDF	666	6.23032e-002	2.77590e-002
	3NBBDF	666	6.98707e-002	2.63337e-002
10^{-3}	1BDF	20,000	1.35548e-002	7.10778e-002
	3BBDF	6,666	3.76165e-002	7.66636e-002
	3NBBDF	6,666	5.40956e-003	2.60816e-001
10^{-4}	1BDF	200,000	1.42927e-003	6.96867e-001
	3BBDF	66,666	4.26516e-003	7.64385e-001
	3NBBDF	66,666	3.08942e-005	2.60725e+000
10^{-5}	1BDF	2,000,000	1.43644e-004	7.703079e+000
	3BBDF	666,666	4.30707e-004	7.63788e+000
	3NBBDF	666,666	3.18534e-007	2.60597e+001
10^{-6}	1BDF	20,000,000	1.43715e-005	6.95855e+001
	3BBDF	6,666,666	4.31123e-005	7.65356e+001
	3NBBDF	6,666,666	3.19872e-009	2.60700e+002

Table 3: Numerical results for problem (3)

h	Method	NS	MAXE	Time
10^{-2}	1BDF	1,000	3.61405e-003	2.44375e-003
	3BBDF	333	1.07308e-002	2.81400e-003
	3NBBDF	333	1.94447e-004	1.20394e-002
10^{-3}	1BDF	10,000	3.67235e-004	2.35480e-002
	3BBDF	3,333	1.10060e-003	5.26718e-001
	3NBBDF	3,333	2.07993e-006	1.19193e-001
10^{-4}	1BDF	100,000	3.67815e-005	2.31844e-001
	3BBDF	33,333	1.10333e-004	2.71459e-001
	3NBBDF	33,333	2.09995e-008	1.19296e+000
10^{-5}	1BDF	1,000,000	3.67873e-006	2.60215e+000
	3BBDF	333,333	1.10361e-005	2.70685e+000
	3NBBDF	333,333	2.10257e-010	1.19173e+001
10^{-6}	1BDF	10,000,000	3.67839e-007	2.31472e+001
	3BBDF	3,333,333	1.10363e-006	2.71178e+001
	3NBBDF	3,333,333	1.41029e-011	1.19110e+002

From the tables above, the accuracy of the new method developed can be clearly seen from the maximum error (MAXE). For all the problems tested, the method is seen to have outperformed the 1BDF and the 3BBDF methods. As an added advantage, our method also reduced the number of steps taken to complete the integration by the 1BDF method to almost $\frac{1}{3}$. However, the computation time of our method is not better than that in the 1BDF and the 3BBDF.

7. CONCLUSION

An implicit method is developed that is suitable for solving stiff ODEs. The method produces 3–solution values simultaneously. The order of the method is 5 and the error constant is seen to be small. A comparison is made with other classes of methods in the BDF family and the accuracy of the method is seen to be better.

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