ENHANCED 3-POINT FULLY IMPLICIT SUPER CLASS OF BLOCK BACKWARD DIFFERENTIATION FORMULA FOR SOLVING STIFF INITIAL VALUE PROBLEMS


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ABSTRACT
This paper modified an existing 3–point block method for solving stiff initial value problems. The modification leads to the derivation of another 3 – point block method which is suitable for solving stiff initial value problems. The method approximates three solutions values per step and its order is 5. Different sets of formula can be generated from it by varying a parameter $\rho \in (-1, 1)$ in the formula. It has been shown that the method is both Zero stable and A–Stable. Some linear and nonlinear stiff problems are solved and the result shows that the method outperformed an existing method and competes with others in terms of accuracy.


INTRODUCTION
Most physical problems in science and engineering are formulated as ordinary differential equations (ODEs). For example, problems in electrical circuits, mechanics, vibrations, chemical reactions, kinetics and population growth can all be modeled by differential equations. Such differential equations can be categorized into stiff and non stiff. Majority of both categories cannot be solved analytically and hence the use of suitable numerical schemes is advocated. Stiff differential equations describe equations where different physical phenomena acting on different time scales occur simultaneously. According to Curtiss and Hirschfelder (1952), implicit numerical schemes proved to be more efficient in solving stiff problems than explicit ones. Most common implicit algorithms are based on Backward Differentiation Formula (BDF). The BDF first appeared in the work of (Curtiss & Hirschfelder, 1952). Researchers continued to improve on the BDF methods. Such improvements include the Extended Backward Differential Formula by (Cash 1980), modified extended backward differential formula by (Cash 2000), block backward differentiation formula (BBDF) by (Ibrahim et al. 2007), 2 point diagonally implicit super class of backward differentiation formula by (Musa et al. 2016), diagonally implicit block backward differentiation formula for solving ODEs by (Zawawi & et al. 2012), a new variable step size block backward differentiation formula for solving stiff initial value problems (Suleiman et al. 2013), a new fifth order implicit block method for solving first order stiff ordinary differential equations by (Musa et al. 2014), a new super class of block backward differentiation formula for stiff ordinary differential equations by Suleiman et al (2014).

This paper extends the work in (Musa et al. 2014) by introducing a non zero coefficient, namely $\beta_{k-2}$. The proposed block method is intended to solve stiff initial value problems (IVPs) by computing three solution values at a time.

Derivation of the Method
Consider the following fifth order implicit block method for solving first order stiff ordinary differential equations developed by (Musa et al. 2014):

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

where ‘$p$’ is a free parameter in the interval (-1, 1) and $\beta_{k-1,i} = \rho \beta_{k,i}$ (see Kanaka (1985)). In formula (1), $\beta_{0,i} = \beta_{1,i} = \hdots = \beta_{k-2,i} = 0$. But $\beta_{k-1,i} \neq 0$, $k = i = 1$, $k = i = 2$ and $k = i = 3$ represent the first, second and third points formula respectively.

In contrast to (1), this paper considers $\beta_{0,i} = \beta_{1,i} = \hdots = \beta_{k-3,i} = \beta_{k-1,i} = \beta_{k-2,i} = 0$; but $\beta_{k-2,i} \neq 0$ where $\beta_{k-2,i} = \rho \beta_{k,i}$. This leads to the new formula:

$$\sum_{i=0}^{5} \alpha_{i,j} y_{n+j-i} = \beta_{k,i} (f_{n+k} - Pf_{n+k-2}), \quad k = i = 1, 2, 3 \quad (2)$$
where \( p \) is considered with the same interval of (-1, 1) as in (Musa et al., 2014).

The implicit method (2) is constructed using a linear operator. To derive the three point formula, define a linear operator \( L_i \) associated with (2) by:

\[
L_i[y(x_n), h]: a_0y'_{n-2} + a_{1,i}y_{n-1} + a_{2,i}y_n + a_{3,i}y_{n+1} + a_{4,i}y_{n+2}\alpha_5y_{n+3} - h^2_0 k_1(f_{n+k} - pf_{n-k-2}) = 0,
\]

\( k = i = 1,2,3 \).

To derive the first point \( y_{n+1} \), substitute \( k = 1 \) in (3) to obtain

\[
L_1[y(x_n), h]: a_0y'_{n-2} + a_{1,1}y_{n-1} + a_{2,1}y_n + a_{3,1}y(x_n) + a_{4,1}y(x_n + h) + a_{5,1}y(x_n + 3h) - h^2_1,1 \left( f_{n+1} - pf_{n-1} \right) = 0
\]

(4)

Expand (4) using Taylor series about \( x_n \) and collect like terms to get

\[
C_{0,0}y_n + hC_{1,0}y_n' + h^2C_{2,0}y_n'' + h^3C_{3,0}y_n''' + ... = 0
\]

(5)

where

\[
C_{0,0} = \alpha_{0,0} + \alpha_{1,0} + \alpha_{2,0} + \alpha_{3,0} + \alpha_{4,0} + \alpha_{5,0} = 0
\]

\[
C_{1,0} = -2\alpha_{0,1} - \alpha_{1,1} + \alpha_{3,1} + \alpha_{4,1} + \alpha_{5,1} = 0
\]

\[
C_{2,0} = 2\alpha_{0,2} + \frac{1}{2}\alpha_{1,2} + \frac{1}{2}\alpha_{2,2} + 2\alpha_{4,1} + 3\alpha_{5,1} + \beta_{1,1}(p - 1) = 0
\]

\[
C_{3,0} = \frac{4}{3}\alpha_{0,3} - \frac{1}{6}\alpha_{1,3} + \frac{1}{6}\alpha_{2,3} + \frac{4}{3}\alpha_{4,1} + \frac{2}{3}\alpha_{5,1} + \frac{1}{2}\beta_{1,1}(p - 1) = 0
\]

\[
C_{4,1} = \frac{2}{3}\alpha_{0,4} + \frac{1}{3}\alpha_{1,4} + \frac{1}{3}\alpha_{2,4} + \frac{2}{3}\alpha_{4,1} + \frac{1}{3}\alpha_{5,1} + \frac{2}{3}\beta_{1,1}(p - 1) = 0
\]

\[
C_{5,0} = -\frac{4}{15}\alpha_{0,5} - \frac{1}{12}\alpha_{1,5} + \frac{1}{12}\alpha_{2,5} + \frac{4}{15}\alpha_{4,1} + \frac{1}{15}\alpha_{5,1} + \frac{1}{24}\beta_{1,1}(p - 1) = 0
\]

\( a_{3,1} \), the coefficient of the first point \( y_{n+1} \), is normalised to 1. Equation (6) is solved simultaneously and the values of the coefficients are substituted into (4) to obtain the first point as:

\[
y_{n+1} = \frac{1}{60}y'_{n-2} + \frac{1}{30}y'_{n-1} + \frac{1}{30}y_n + \frac{2}{30}y_{n+1} - \frac{1}{20}f_{n+1} - \frac{3}{20}f_{n-1}
\]

(7)

To derive the second and the third points, substitute \( k = 2 \) and \( k = 3 \) respectively in (3) and follow similar procedure as described in the derivation of the first point. The three point block method is therefore obtained as:

\[
y_{n+2} = \frac{1}{60}y'_{n-2} + \frac{1}{30}y'_{n-1} + \frac{1}{30}y_n + \frac{2}{30}y_{n+1} - \frac{1}{20}f_{n+1} - \frac{3}{20}f_{n-1}
\]

\[
y_{n+3} = \frac{2}{60}y'_{n-2} + \frac{1}{30}y'_{n-1} + \frac{1}{30}y_n + \frac{2}{30}y_{n+1} - \frac{1}{20}f_{n+1} - \frac{3}{20}f_{n-1}
\]

(8)

In this paper, formula (8) is called ‘Enhanced 3-Point Fully Implicit Super Class of Block Backward Differentiation Formula (EBD3BBF)’ for solving stiff initial value Problems. For stability reasons, the value of the free parameter \( p \) is restricted within the interval (-1, 1) as in (Musa et al., 2014) and (kanaka 1985). The proof of the stability of BBD method of the form \( \sum_{i=0}^{3} a_{i}y_{n+i} = h^2 k_1(f_{n+k} - pf_{n-k-2}) \) can be found in (kanaka 1985). Substituting \( \rho = -\frac{2}{5} \) in (8), the E3BBDF is obtained as:

\[
y_{n+1} = \frac{27}{625}y'_{n-2} + \frac{27}{625}y'_{n-1} + \frac{27}{625}y_{n} + \frac{27}{625}y_{n+1} - \frac{9}{625}f_{n+1} - \frac{7}{625}f_{n-1}
\]

\[
y_{n+2} = \frac{27}{625}y'_{n-2} + \frac{27}{625}y'_{n-1} + \frac{27}{625}y_{n} + \frac{27}{625}y_{n+1} - \frac{9}{625}f_{n+1} - \frac{7}{625}f_{n-1}
\]

\[
y_{n+3} = \frac{68}{673}y'_{n-2} + \frac{68}{673}y'_{n-1} + \frac{68}{673}y_{n} - \frac{68}{673}y_{n+1} + \frac{68}{673}y_{n+2} + \frac{68}{673}y_{n+3} + \frac{68}{673}f_{n+1} + \frac{68}{673}f_{n-1}
\]

(9)

Stability Analysis

Definition (Zero stability)

A linear multi-step method is said to be zero stable if all the roots of first characteristics polynomial have modulus less than or equal to unity and those roots with modulus unity are simple.

The method (9) can be written in matrix form as

\[
\begin{pmatrix}
1 & -\frac{23}{14} & \frac{27}{14} \\
-\frac{27}{55} & 1 & \frac{265}{673} \\
-\frac{1380}{673} & \frac{1380}{673} & 1
\end{pmatrix}
\begin{pmatrix}
y_{n+1} \\
y_{n+2} \\
y_{n+3}
\end{pmatrix}
= \begin{pmatrix}
\frac{29}{70} & -\frac{37}{28} & \frac{9}{7} \\
-\frac{27}{265} & \frac{44}{53} & \frac{53}{53} \\
\frac{68}{673} & \frac{68}{673} & \frac{1240}{673}
\end{pmatrix}
\begin{pmatrix}
y'_{n} \\
y'_{n-1} \\
y'_{n-2}
\end{pmatrix}
\]

\( \begin{pmatrix}
y_{n-1} \\
y_{n-2} \\
y_{n-3}
\end{pmatrix}
\)
Equation (10) can be rewritten in the following form:

\[ A_0 Y_m = A_1 Y_{m-1} + h(B_0 F_{m-1} + B_1 F_m) \]  

(11)

where

\[
A_0 = \begin{pmatrix}
1 & \frac{-23}{14} & \frac{27}{140} \\
\frac{-27}{140} & 1 & \frac{68}{265} \\
\frac{1580}{265} & \frac{-1300}{265} & -1
\end{pmatrix}, \quad
A_1 = \begin{pmatrix}
\frac{-29}{70} & \frac{-37}{70} & 0 \\
\frac{27}{673} & \frac{44}{673} & \frac{53}{673} \\
\frac{1580}{673} & \frac{-1300}{673} & \frac{673}{673}
\end{pmatrix}, \quad
B_0 = \begin{pmatrix}
0 & \frac{-12}{27} & 0 \\
0 & 0 & \frac{68}{265} \\
0 & 0 & -1
\end{pmatrix}, \quad
B_1 = \begin{pmatrix}
\frac{-15}{240} & 0 & 0 \\
0 & \frac{68}{265} & 0 \\
\frac{240}{265} & 0 & \frac{100}{265}
\end{pmatrix}.
\]

Substituting the scalar test equation

\[ y' = \lambda y \]

(\( \lambda < 0, \lambda \) complex) into (11) and using \( \lambda h = \bar{h} \) gives

\[ A_0 Y_m = A_1 Y_{m-1} + \bar{h}(B_0 F_{m-1} + B_1 F_m) \]

(13)

The stability polynomial of (9) is obtained by evaluating

\[ \text{De}(A_0 - \bar{h}B_1) \lambda - (A_1 + \bar{h}B_0) = 0 \]

(14)

to obtain the following first characteristic polynomial:

\[
R(\bar{h}, t) = \frac{63882}{35669} t^3 + \frac{46296}{249683} t^2 + \frac{6959103}{4244611} t + \frac{7267896}{606373} \bar{h} + \frac{3667896}{249683} t^2 \bar{h} + \frac{7267896}{606373} t^2 \bar{h}^2 - \frac{7267896}{606373} t^3 \bar{h} + \frac{720920}{249683} t^3 \bar{h}^2 - \frac{270000}{606373} t^3 \bar{h}^3 + \frac{2449683}{249683} \bar{h}^2 - \frac{2449683}{249683} \bar{h}^3 - \frac{138240}{249683} t^3 \bar{h}^3 - \frac{402210}{249683} t^3 + \frac{142767}{249683} t^3 = 0
\]

(15)

By substituting \( \bar{h} = 0 \) in (15), the first characteristic polynomial is obtained as:

\[
R(t, 0) = \frac{402210}{249683} t^3 + \frac{7267896}{249683} t^2 + \frac{63882}{35669} t + \frac{142767}{249683} = 0
\]

(16)

Solving (16) for \( t \) gives the roots as: \( t = 1, t = 0.8385877317, \text{and} \ t = -0.0817517514 \). Therefore by definition above, the method is Zero Stable.

**Definition (A-stability)**

A linear multi-step method is said to be A-stable if the stability region covers the entire negative half plane.

The stability region of the method (9) is shown in the following figure:

**Figure: 1:** Stability Region of the Method when \( \rho = -\frac{4}{5} \)

The stability region is the region outside the circular shape, and thus covered the entire negative half plane. Thus, by the definition of A-stability stated above, the method is A-stable. Hence, the method is both Zero and A-stable, it is suitable for solving stiff initial value problems.
Implementation of the Method
Applying Newton’s iteration let \( y_i \) and \( y_i(x_i) \) be the approximate and exact solutions respectively of the stiff IVP:
\[
y' = f(x, y), \quad y(x_0) = y_0, \quad x \in (a, b)
\]  \hfill (17)
Define the error as:
\[
(error)_i = |(y_i)_i - (y(x_i))_i|
\]  \hfill (18)
and the maximum error as:
\[
MAXE = \max_{1 \leq i \leq N} (\max(error)_i).
\]
where \( T \) is the total number of steps and \( N \) is the number of equations (see Ibrahim et al. (2007)).
Define
\[
F_1 = y_{n+1} + \frac{1}{2160}y_{n+2} + \frac{22}{945}y_{n+3} + \frac{1}{252}y_{n+1} - \frac{6}{7}f_1 + \frac{2}{252}f_2 - \frac{1}{504}e_1 - e_3
\]
\[
F_2 = y_{n+2} - \frac{2}{2160}y_{n+2} + \frac{1}{945}y_{n+3} - \frac{1}{252}y_{n+1} - \frac{2}{252}f_1 + \frac{1}{504}e_1 - e_3
\]
\[
F_3 = y_{n+3} + \frac{1}{2160}y_{n+2} + \frac{22}{945}y_{n+3} - \frac{1}{252}y_{n+1} - \frac{2}{252}f_1 + \frac{1}{504}e_1 - e_3
\]  \hfill (19)
where \( e_1, \ e_2 \) and \( e_3 \) are the back values obtained from the method (9) as:
\[
e_1 = \frac{11}{27}y_{n-1} - \frac{8}{27}y_{n} + \frac{1}{27}y_{n+1}
\]
\[
e_2 = \frac{2}{27}y_{n-1} + \frac{5}{27}y_{n} - \frac{3}{27}y_{n+1}
\]  \hfill (20)
\[
e_3 = \frac{14}{27}y_{n-1} - \frac{10}{27}y_{n} + \frac{1}{27}y_{n+1}
\]
The Newton’s iteration takes the form
\[
y_{i+1} = y_i + \frac{1}{F_i(y)} \left[ F'_i(y) \right]^{-1}
\]  \hfill (21)
Hence, (21) can be written as
\[
[F'_i(y)]e_{i+1} = -F_i(y)
\]  \hfill (22)
Equation (22) is equivalent to:
\[
\begin{pmatrix}
1 + \frac{17}{72}y_{n+1} & -\frac{23}{72} & \frac{7}{72} \\
-\frac{60}{72} y_{n+2} & 1 & -\frac{68}{72} \\
\frac{180}{72} y_{n+3} & \frac{265}{72} & -1
\end{pmatrix}
\begin{pmatrix}
\epsilon_{n+1}^{(i+1)} \\
\epsilon_{n+2}^{(i+1)} \\
\epsilon_{n+3}^{(i+1)}
\end{pmatrix}
= \begin{pmatrix}
\begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix} + \frac{10}{72} \begin{pmatrix}
y_n^- \\
y_n^- \\
y_n^+ - 1
\end{pmatrix} + \frac{10}{27} \begin{pmatrix}
y_{n+1}^- \\
y_{n+2}^- \\
y_{n+3}^-
\end{pmatrix}
\end{pmatrix}
\]  \hfill (23)
A computer programming is designed to implement (23)

1. Test Problems
To validate the method developed, the following stiff IVPs are solved. Problem 1 is a non-linear while problems 2 and 3 are linear.

Problem 1: \( y' = 5e^{5x}(y - x)^2 + 1 \quad y(0) = 0 \quad 0 \leq x \leq 1 \)

Exact solution:
\( y(x) = x - e^{-5x} \)
Source: (Lee et al., 2002)

Problem 2: \( y'_1 = -20y_1 - 19y_2 \quad y_1(0) = 2 \quad 0 \leq x \leq 20 \)
\( y'_2 = -19y_1 - 20y_2 \quad y_2(0) = 0 \)

Exact solution:
\( y_1(x) = e^{-39x} + e^{-x} \)
\( y_2(x) = e^{-39x} - e^{-x} \)
Source: (Cheney & Kincaid2012)

Problem 3: \( y'_1 = 198y_1 + 199y_2 \quad y_1(0) = 1 \quad 0 \leq x \leq 10 \)
\( y'_2 = -39y_1 - 399y_2 \quad y_1(0) = -1 \)

Exact solution:
\( y_1(x) = e^{-x} \)
\( y_2(x) = -e^{-x} \)
Eigenv values -1 and -200
Numerical Result
The problems presented in section 5 are solved using the developed method and some other methods available in the literature. The results are compared in tables; and graphs depicting the performance of each method are plotted. The following notations are used in the tables:

- $h = \text{step-size}$;
- $\text{NS} = \text{Number of steps}$
- $\text{MAXE} = \text{Maximum Error}$
- $T = \text{Time in s.}$

3BBDF = 3-Point block backward differentiation formula for solving stiff IVPs.
3NBBDF = A 3-Point New fifth order implicit block Method for solving first order stiff ODEs.
3ESBBDF = 3-Point Enhanced fully implicit Super Class of Block Backward Differentiation Formula for solving Stiff IVPs.

Table 1. Numerical results for problem 1

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<th>Method</th>
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<th>MAXE</th>
<th>TIME</th>
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Table 2. Numerical results for problem 2

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<td>7.59821e+000</td>
</tr>
<tr>
<td>$10^{-6}$</td>
<td>3BBDF</td>
<td>6,666,666</td>
<td>4.31123e-005</td>
<td>7.65356e+001</td>
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<tr>
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<td>3.19872e-009</td>
<td>2.60700e+002</td>
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<td>6.33362e-010</td>
<td>7.53567e+001</td>
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</table>
Table 3. Numerical results for problem 3

<table>
<thead>
<tr>
<th>h</th>
<th>Method</th>
<th>NS</th>
<th>MAXE</th>
<th>TIME</th>
</tr>
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<tbody>
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<td>1.07308e-002</td>
<td>1.37500e-002</td>
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<tr>
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<td>1.20394e-003</td>
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<tr>
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<td>2.72200e-002</td>
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<td>3,333</td>
<td>2.07993e-006</td>
<td>1.25972e-002</td>
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<td>5.81512e-002</td>
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<tr>
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<td>1.25471e+000</td>
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<td>1.10363e-006</td>
<td>1.91700e+001</td>
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</tbody>
</table>

From the Tables 1–3, it can be seen that the 3ESBBDF outperformed the 3BBDF in terms of accuracy and minimum computational time. Also, the 3ESBBDF competes with the 3NBBDF in terms of accuracy. However, the computation time of the new method does not seem to be better in comparison with the other method 3NBBDF for most of the problems solved.

To further compare the performance of the methods, the graphs of $\log_{10}(MAXE)$ against $h$ for the problems tested are plotted and presented as follows:

![Figure 2: Graph of $\log_{10}(MAXE)$ against $h$ for problem 1](image)
Figure 3: Graph of $\log_{10}(MAXE)$ against $h$ for problem 2

Figure 4: Graph of $\log_{10}(MAXE)$ against $h$ for problem 3

The graphs in Figure 2 – 4 also show that the scaled error for the 3ESBBDF is smaller when compared with that in 3BBDF method. However, the 3ESBBDF is competing with 3NSBBDF.

CONCLUSION

A 3–point enhanced fully implicit Super class method (3ESBBDF) has been developed for the solution of first order stiff initial value problems. It is achieved by modifying an existing block method to include a non zero coefficient $\beta_{k-2}$. The developed method is both zero stable and $A$ – stable. There is an improvement in accuracy and minimum computational time of the method (3ESBBDF) when compared with the BBDF method and competes with $3NBBD$ method. Another advantage of the method over the BBDF is that one can vary a parameter within (-1, 1) and still achieve $A$ – stability and better accuracy.
REFERENCES


