Convergence of the 3-point block backward differentiation formulas with off-step point for stiff ODEs

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Abstract. Development of 3-Point Block Method with one off-step point using Backward Differentiation Formula (BDF) is presented in this paper to find out the solution for stiff Ordinary Differential Equation (ODEs). By considering the Backward Differentiation Formulas (BBDF), the block method has been derived. It is well known that BBDF is used for solving stiff ODEs. The strategy for the development of this process is to compute three solution values with one off-step point concurrently to each iteration. One off-step point is added in the implicit BBDF method for better accuracy. Derivation of the formulae and consistency properties are generated in this paper. Numerically the proposed method with order five is achieved as a result. Mathematica software has been used for the derivation and consistency of the method.

1. Introduction
Many real-world problems consist of ordinary differential equations, appears in various fields. Such as modelling process of cooling, radioactive decay, chemical kinetics, biology, economics, geology, economics, physics and various aspects of engineering to approximate the solution as an alternative solver. Therefore, ODEs with first order are getting substantial attention.

Stiffness of the problems are the main issue because these problems comprises of an extensively unpredictable time scale i.e., solutions of some components decomposes more faster than others [1, 2].

Our objective is to derive a multistep 3-point block method with one off-step point, which can solve stiff ODEs efficiently.

Considering the first order ODE,

\[ y'(x) = f(x, y), \quad y'(a) = y_0 \]  

having \( x \in [a, b] \).

To solve the equation (1) the numerical methods are developed by types of ODEs, e.g. non-linear or linear, either stiff or non-stiff ODEs. It should be noted that by using incorrect method for a model may give slow or wrong solution. Mostly, problems having form (1) are categorized into two types. Non-stiff problem is the first type, in which the explicit methods are used along with some error control. Whereas Stiff ODEs are the second type. The word “Stiff” was firstly introduced by [3] in chemical kinetics’ problems. The solutions of stiff problems can only be found by using implicit methods because by using explicit methods it works very slowly or sometimes fails to provide an accurate solution [4]. Stiffness is described in various literature as there is not any specific definition. (1) is said to be explaining the stiff problems if,

i) The Stability region decided on the bases of step size rather than the requirement of accuracy [5];
ii) The stiffness ratio (the ratio of the magnitudes of the real parts of the largest and smallest eigenvalues) is significant and all of its eigenvalues have negative real part [5];

iii) None of the component of solution is unstable (Jacobian matrix having no eigen values which has a real part that is positive and large) and less components are very stable (one an eigenvalue possess real part at least that is negative and large) [6].

Lambert [7] specified the stiffness of (1) as,

\[
\text{Def. 1:}
\]

i) \( \frac{\max_{t=1,2,\ldots,m} |Re(\lambda_{t})|}{\min_{t=1,2,\ldots,m} |Re(\lambda_{t})|} \)

\( \lambda_{t} \) are the eigen values and ratio \( \frac{\max_{t=1,2,\ldots,m} |Re(\lambda_{t})|}{\min_{t=1,2,\ldots,m} |Re(\lambda_{t})|} \) is called stiffness ratio.

Gear [8] firstly introduced the Backward Differentiation Formulas (BDF), that is considered as proficient and well-known for solving extensive problems of stiff ODEs. Various scholars have derived the classical BDF block methods. Ibrahim et Al [9, 10], Yatim et. al [11], Abasi et. al [1] and Zainuddin et. al [12] have presented the extension of block method. Block method are classified into single or multi-step method. Runge-Kutta method is the standard single step method introduced by Rosser [13]. Watts and Shampine [14] researched on A-stable r-block single-step implicit method. Block method having 4\textsuperscript{th} order that is used as a predictor-corrector method for multistep method were proposed by Voss and Abbas [15]. Modified extended BDF method for numerical solutions of still ODEs were proposed by J.R. Cash [16]. Ibrahim et. al [9] developed a method for 2-point and 3-point block BDF for solving first order ODEs. Nasir et.al [17] modified the existing block method by developing the order which is named as 5\textsuperscript{th} order 2-Point Block Backward Differentiation Formula (BBDF). Musa et.al [18] improved the Block BDF method by addition of future points.

This paper is the extension of A.A. Nasaru din, Z.B. Ibrahim and H. Rosali [19] and Abasi et. al [1]. The determination of derivation of 3-Point (3PBBDF) with one off-step point is to get the better approximation of the solution that would be compared with the previous existing methods. Furthermore, convergence property of the method is also been discussed in this paper. The following section will briefly describe the formulation of the method.

2. Derivation of 3-Point Block BDF with one off-step point.

Present section comprises of the derivation of three solution values \( y_{n+1}, y_{n+2} \) and \( y_{n+3} \) having step size \( h \) with one off-step point \( y_{n+1/2} \) in which half of the step size is shaped up in a block. By using two back values \( y_{n-1} \) and \( y_{n} \) in the previous block (Figure 1), these formulas will be computed with \( h \) step size. Numerous points have been examined for choosing the suitable off-step point. After some observation, it has been noticed that the halved step size helps to acquire the desired stability and optimized point formula [1].

![Figure 1. 3-Points Block with one off step point](image-url)
To interpolate the values of $y$ at $(x_{n-1}, y_{n-1})$, $(x_n, y_n)$, $(x_{n+1}, y_{n+1})$, $(x_{n+2}, y_{n+2})$, $(x_{n+5}, y_{n+5})$ and $(x_{n+3}, y_{n+3})$, Lagrange interpolation formula has been used that is well-defined as,

$$P_k(x) = \sum_{j=0}^{k} L_{k,j}(x)y(x_{n+3-j})$$

Where

$$L_{k,j} = \prod_{\substack{i=0\atop i \neq j}}^{k} \frac{x-x_{n+3-i}}{x_j-x_{n+3-i}}$$

for $j = 0, 1, 2, \ldots, k$

$$P(x) = \frac{(x-x_{n-1})(x-x_n)(x-x_{n+1})(x-x_{n+2})(x-x_{n+3})}{(x_{n+3}-x_{n-1})(x_{n+3}-x_n)(x_{n+3}-x_{n+1})(x_{n+3}-x_{n+2})(x_{n+3}-x_{n+3})} \times y(x_{n+3})$$

$$+ \frac{(x-x_{n-1})(x-x_n)(x-x_{n+1})(x-x_{n+2})}{(x_{n+3}-x_{n-1})(x_{n+3}-x_n)(x_{n+3}-x_{n+1})(x_{n+3}-x_{n+2})(x_{n+3}-x_{n+3})} \times y(x_{n+3})$$

$$+ \frac{(x-x_{n-1})(x-x_n)(x-x_{n+1})(x-x_{n+2})}{(x_{n+3}-x_{n-1})(x_{n+3}-x_n)(x_{n+3}-x_{n+1})(x_{n+3}-x_{n+2})(x_{n+3}-x_{n+3})} \times y(x_{n+2})$$

$$+ \frac{(x-x_{n-1})(x-x_n)(x-x_{n+1})(x-x_{n+2})}{(x_{n+3}-x_{n-1})(x_{n+3}-x_n)(x_{n+3}-x_{n+1})(x_{n+3}-x_{n+2})(x_{n+3}-x_{n+3})} \times y(x_{n+1})$$

$$+ \frac{(x-x_{n-1})(x-x_n)(x-x_{n+1})(x-x_{n+2})}{(x_{n+3}-x_{n-1})(x_{n+3}-x_n)(x_{n+3}-x_{n+1})(x_{n+3}-x_{n+2})(x_{n+3}-x_{n+3})} \times y(x_{n})$$

$$+ \frac{(x-x_{n-1})(x-x_n)(x-x_{n+1})(x-x_{n+2})}{(x_{n+3}-x_{n-1})(x_{n+3}-x_n)(x_{n+3}-x_{n+1})(x_{n+3}-x_{n+2})(x_{n+3}-x_{n+3})} \times y(x_{n-1})$$

Where as $s = \frac{x-x_{n+1}}{h}$ and then substitute $x = x_{n+1} + sh$ in the (3), hence,

$$P(x_{n+1} + sh) = \frac{(sh+h)(sh+h)(sh+h)(sh-2h)}{(3h)(3h)(3h)(3h)} \times y(x_{n+3}) + \frac{(sh+h)(sh)(sh)(sh-2h)}{(2h)(2h)(2h)(2h)} \times y(x_{n+2})$$

$$+ \frac{(sh+h)(sh)(sh)(sh-2h)}{(h)(h)(h)(h)} \times y(x_{n+1})$$

Differentiating (4) with respect to $s$ expanded as

$$P(x_{n+1} + sh) = \frac{y_{n+1}}{12} \left[ (s+2)(s+1)(s-1) \left( s - \frac{3}{2} \right) + \frac{32y_{n+5}}{15} \right]$$

$$+ \frac{y_{n+2}}{3} \left[ (s+2)(s+1)(s-1) \left( s - \frac{3}{2} \right) + \frac{15y_{n-1}}{(s+1)(s-1)(s-\frac{3}{2})} \right]$$

$$+ \frac{y_{n}}{15} \left[ (s+2)(s-1) \left( s - \frac{3}{2} \right) + \frac{y_{n-1}}{84} \right]$$
Expanding (5) and afterward proceeded by differentiating with respect to s. substituting s with 0, 1, 3/2, and 2 gives the formulas for the points \( y_{n+1}, y_{n+2}, y_{n+3/2}, \) and \( y_{n+3} \) with constant step size.

Finally, the set of formulae of 3BBDF with off step point is given as,

\[
\begin{align*}
y_{n+1} &= \frac{3}{56} y_{n+1} - \frac{3}{5} y_n + 3 y_{n+2} - \frac{64}{35} y_{n+2}^5 + \frac{3}{8} y_{n+3} - \frac{3}{2} h^2 f_{n+1} \\
y_{n+2} &= -\frac{1}{98} y_{n+1} - \frac{3}{35} y_n - \frac{1}{7} y_{n+1} + \frac{384}{245} y_{n+2} - \frac{3}{14} y_{n+3} - \frac{6}{7} h^2 f_{n+2} \\
y_{n+3} &= -\frac{75}{9080} y_{n+1} + \frac{147}{2272} y_n - \frac{1225}{4544} y_{n+1} + \frac{3675}{2272} y_{n+2} - \frac{3675}{9080} y_{n+3} + \frac{105}{142} h^2 f_{n+2} \\
y_{n+3} &= -\frac{3}{343} y_{n+1} - \frac{16}{245} y_n + \frac{12}{49} y_{n+1} - \frac{48}{49} y_{n+2} + \frac{3072}{1715} y_{n+2}^5 + \frac{12}{49} h^2 f_{n+3}
\end{align*}
\]

(6)

In the next section convergence property of the derived 3-Point BBDF method has been discussed.

3. Convergence of the method

The linear multistep method (LMM) is acceptable if the method’s solution converges, to the theoretical solution as the step-length \( h \) approaches to zero. If the term “convergent” is to be applied to the equation

\[
\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}
\]

Then the convergence property must hold for all initial values problems (1).

A. Required Conditions for Convergence
1. It must be zero-stable.
2. And it must be consistent.
   a. Consistency

If (7) holds order \( p \geq 1 \) then it is said to be consistent. The method (6) is consistent if and only if

\[
\sum_{j=0}^{k} \alpha_j = 0 \quad \text{and} \quad \sum_{j=0}^{k} j \alpha_j = \sum_{j=0}^{k} \beta_j
\]

b. Stability

The method is computationally practical if it has a region of absolute stability which will assure that the method is able to solve stiff problems.

Starting with the definition of zero stability and A-stability (lambert 1973).

Def. 1. (Zero stable): The (7) is zero stable if 1st characteristics of the polynomial possess no root with modulus greater than one, also each root with modulus one is simple.

Def. 2. (A-stable): The method is A-stable if for all \( \lambda \) in the left-half plane (Re(\( \lambda \)) \leq 0). In which whole negative left-half plane is covered to display the stability region.
3.1. Order and Error constant of the 3-point BBDF with one off-step point

In this section, we are formulating the Taylor series method, for finding out the order by using LMM. With (7), we co-relate the linear difference operator as

$$L[y(x_n); h] = \sum_{j=0}^{k+5-1} \alpha_j (x_{n+j-1})_y(x_n + Th) - h \beta \delta_T y(x_n + Th)$$  \hspace{1cm} (8)

where an arbitrary constant y, is continuous and differentiable function [20].

The general linear multistep method for 3-point BBDF with one off-step point is defined by:

$$\sum_{j=0}^{k+5-1} \alpha_j (x_{n+j-1})_y = h \beta \delta_T f_{n+T}$$  \hspace{1cm} (9)

The function $y(x + Th)$ is expanded with its derivative $y'(x + Th)$, and gathering terms in (8) will get,

$$L = [y(x); h] = C_0 y(x) + C_1 y'(x) + \ldots + C_q h^q y^{(q)} (x) + \ldots$$  \hspace{1cm} (10)

$C_q$ are the constants and vary from function to function.

Def. 3: The difference operator (8) and the related LMM (9) are supposed to be order $p$ if, in (10), $C_0 = C_1 = \ldots = C_p = 0$ and $C_{p+1} \neq 0$.

Following formulae are used to find out the constant $C_q$ in terms of $\alpha_j$ and $\beta_j$

- $C_0 = \alpha_0 + \alpha_1 + \alpha_2 + \ldots + \alpha_k$
- $C_1 = \alpha_0 + 2\alpha_1 + \alpha_2 + \ldots + k\alpha_k - (\beta_0 + \beta_1 + \beta_2 + \ldots + \beta_k)$
- $\vdots$
- $C_q = \frac{1}{q!}(\alpha_0 + 2^q\alpha_2 + \ldots + k^q\alpha_k) - \frac{1}{(q-1)!}(\beta_0 + 2^{q-1}\beta_2 + \ldots + k^{q-1}\beta_k)$

The order for the given method can be derived by using formulas (11). By using formulas (11) for all four cases, we got

$$C_5 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

but $C_6 \neq 0$. Hence, it shows that the order of 3-Point BBDF method with one off-step point is 5 and the error constant is,

$$C_6 = \begin{bmatrix} 1 \\ 180 \\ -280 \\ 6250 \\ -245 \end{bmatrix}$$

3.2. Stability of the 3-Point Block BDF with one off-step point

Specifications for stability of the method is examine in this section. $y' = \lambda y$, $\lambda < 0$, is the scalar test will be applied to the (6).
\[ y_{n+3} = \frac{3}{49} y_{n+1} - \frac{12}{49} y_{n+2} + \frac{3072}{1715} y_{n+3} + \frac{12}{49} h^3 y_{n+3} \]

The formulas (12) are then inscribed into the matrix form to attain the matrix as follows

\[
\begin{bmatrix}
\frac{3}{8} & \frac{64}{35} & -3 & 1 + \frac{3}{2} h \lambda \\
3 & -384 & 1 + \frac{6}{7} h \lambda & \frac{3}{7} \\
\frac{14}{3675} & \frac{105}{9088} & \frac{105}{9088} & \frac{1225}{4544} \\
1 - \frac{12}{49} h \lambda & \frac{142}{3072} & - \frac{2272}{48} & \frac{16}{49}
\end{bmatrix}
\begin{bmatrix}
y_{n+3} \\
y_{n+2} \\
y_{n+1} \\
y_{n+1}
\end{bmatrix}
= \begin{bmatrix}
\frac{3}{5} & 0 & \frac{3}{56} & 0 \\
0 & 0 & 1 & 0 \\
\frac{147}{35} & 0 & - \frac{98}{7} & 0 \\
- \frac{245}{16} & 0 & 3 & 0
\end{bmatrix}
\begin{bmatrix}
y_{n} \\
y_{n-1} \\
y_{n-2} \\
y_{n-2}
\end{bmatrix}
\]

Equation (12) is equivalent to,

\[ A Y_n = B Y_{n-1} \quad (13) \]

where \( H = h \lambda \) is evaluated for the stability polynomial \( R(t,H) \) by \( |At-B| \) as

\[
R(t,H) = \frac{-13977 t^2}{79147250} + \frac{44523 H t^2}{156294500} - \frac{9 H^2 t^2}{179199 H^4 t^4} + \frac{2883852 t^3}{344125} - \frac{811134 H t^3}{48706} - \frac{15070599 H^2 t^3}{39573625} - \frac{9899 H^3 t^3}{48706} + \frac{41616 t^4}{48706}
\]

we set \( H=0 \) in (14) for zero-stability to get the first characteristic polynomial

\[ R(t,0) = \frac{-13977 t^2}{79147250} + \frac{2883852 t^3}{344125} + \frac{41616 t^4}{48706} \quad (15) \]

Solving (14) for \( t \), gives \( t=0, t=-0.000186375, t=0.999767 \). As all the roots of (14) satisfies the condition presented in Def. 1, hence the scheme is zero-stable. Figure 2 shows the stability region of the given method.

![Figure 2. Stability region of the 3-point BBDF (5) method](image)
4. Results and conclusion
A technique which yields a method with continuous coefficients has been presented for the approximated solution for first order ODEs with initial conditions. In this paper, we have derived the 3PBBDF having one off-step point for solving the system of stiff ODEs with constant step size.

Additionally, the order of the 3PBBDF along with one off-step point method is also derived. The stability of the method is also been analyzed by using Mathematica software. As a whole, we can conclude that the order of 3-Point BBDF method is 5 and a zero-stable method. As the 3PBBDF with off-step point acquires the order $p > 1$, therefore is it consistent.

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