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Three-step optimized block backward differentiation formulae (TOBBDF) for solving stiff ordinary differential equations

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A three-step optimized block backward differentiation formulae for solving stiff ordinary differential equations of first-order differential equations is presented. The method adopts polynomial of order 6 and three hybrid points chosen appropriately to optimize the local truncation errors of the main formulas for the block. The method is zero-stable and consistent with sixth algebraic order. Some numerical examples were solved to examine the efficiency and accuracy of the proposed method. The results show that the method is accurate.

Key words: Three-step, optimized block backward differentiation formulae, stiff, zero stable, consistent, convergent, first-order.

INTRODUCTION

A differential equation can be defined as an equation that creates a relationship between an unknown function and one or more of its derivatives. In other words, it is a relationship existing between a dependent variable and one or more independent variable (Dahlquist, 1956). Block methods for solving ordinary differential equations were proposed by Milne (1953). He has some drawbacks such as low order of accuracy, error term and poor performance and this led to the introduction of hybrid methods. Hybrid methods were initially introduced to overcome zero-stability barrier that occurred in block methods as can be seen in Dahlquist (Dahlquist, 1956). Besides the ability to change step size, the other benefit of these methods is utilizing data off-step points which

contribute to the accuracy of the methods.

This paper presents a three-step optimized block backward differentiation formula for the numerical solution of stiff first-order differential equations. The basic properties of the methods such as zero stability, order, consistency, and convergence were examined. Several numerical problems will be solved and comparison will be made with other methods to show the efficiency of the proposed method (Table 1). This paper considers an approximate method for the solution of stiff differential equation of first-order initial value problem of the form,

$$y' = f(x, y), y(t_0) = y_0, \quad (1)$$

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Table 1. The exact solution, the computed solution and the error in the developed method for Problem 1.

X	Exact solution	Computed solution	Error in our method
0.01	0.9048374180	0.9048374180	0.00000
0.02	0.8187307531	0.8187307530	1.000000(-010)
0.03	0.7408182207	0.7408182205	2.000000(-010)
0.04	0.6703200460	0.6703200458	2.000000(-010)
0.05	0.6065306597	0.6065306595	2.000000(-010)
0.06	0.5488116361	0.5488116358	3.000000(-010)
0.07	0.4965853038	0.4965853035	3.000000(-010)
0.08	0.4493289641	0.4493289638	3.000000(-010)
0.09	0.4065696597	0.4065696594	3.000000(-010)
0.10	0.3678794412	0.3678794408	4.000000(-010)

where (x, y) is continuous and satisfies the existence and uniqueness theorem (Henrici, 1962). Recently many authors have applied hybrid block method with a different number of steps and hybrid points to find numerical solutions for the first-order differential equations (Sagir, 2014; Raymond et al., 2018; Ramos, 2017; Areo and Adeniyi, 2014; Yakusak and Adeniyi, 2015; Yahaya and Tijjani, 2015; Fotta and Alabi, 2015; Sunday et al., 2015). In this paper, we optimized the local truncation errors to find three off-points in one step to obtain the most accurate solution.

The algorithm presented in this paper is based on block method and approximates the solution at several points (Raymond et al., 2018; Olanegan et al., 2015; Areo and Adeniyi, 2014; Yakusak and Adeniyi, 2015). Block methods were first introduced by Yahaya and Tijjani (2015) as a means of obtaining starting values for predictor-corrector algorithms and has since then been developed by several researchers (Milne, 1953; Fotta and Alabi, 2015; Sunday et al., 2015; Odejide and Adeniran, 2012), for general use. This paper presents a block method which preserves the Runge-Kutta traditional advantage of being self-starting and efficient.

Definition 1: Stiff equations

A stiff equation is a differential equation that is characterized as that whose exact solution has a term of the form, e^{-cx} where c is a large positive constant (Sunday et al., 2015).

Definition 2: Step-length or mesh-size

A numerical method for solving the differential equation is based on the principle of discretization in which the approximate solutions are evaluated at each grid point. We consider the sequence of points $\{x_n\}$ in the interval $I = [a, b]$ defined by $a = x_0 < x_1 < x_2, \dots, < x_n = b$

; $h_i = x_{i+1} - x_i$, $i = 0(1)n - 1$. The parameter h_i is called the step-size. If the solution, $y(x)$ to a linear multistep method is approximated by y_{n+i} , $i = 0(1)k$, then any numerical method that computes y_{n+i} by using the information at $x_i, x_{i+1}, \dots, x_{n+k}$ is called a K - step method.

Definition 3: Maximal order

A linear multistep method is said to be of maximal order if it has order $2k$ when k is even and order $2k - 1$ when k is odd ($k = \text{step-length}$)

Definition 4: Interval of periodicity

A linear multistep method, when applied to a problem $y^n = \lambda y$, $\lambda > 0$, n represents the the order of the differential equation, is said to have interval of periodicity $(0, h)$, if all the roots of $\rho(\varepsilon) + h\sigma(\varepsilon) = 0$ are complex and lie on a unit circle.

Definition 5: P-stability

A linear multistep method is said to be p -stable if its interval of periodicity is $(0, \infty)$

Definition 6: A-stability

A linear multistep method is said to be A -stable if its interval of periodicity is $(-\infty, 0)$.

MATHEMATICAL DERIVATION OF THE METHODS

Here, we construct the main method and additional

Table 2. Comparison of the newly developed method with Raymond et al. (2018)

X	Exact solution	Computed solution	Error in our method	Raymond et al (2018)
0.01	0.9900498337	0.9900498338	1.000000(-010)	1.959599 (-011)
0.02	0.9801986733	0.9801986733	0.000000	2.477574 (-009)
0.03	0.9704455335	0.9704455335	0.000000	4.181828 (-008)
0.04	0.9607894392	0.9607894392	0.000000	3.095199 (-007)
0.05	0.9512294245	0.9512294244	1.000000(-010)	1.458543 (-006)
0.06	0.9417645336	0.9417645335	1.000000(-010)	1.319575 (-006)
0.07	0.9323938199	0.9323938199	0.000000	1.197493 (-006)
0.08	0.9231163464	0.9231163463	1.000000(-010)	1.105731 (-006)
0.09	0.9139311853	0.9139311851	2.000000(-010)	1.165290 (-006)
1.00	0.9048374180	0.9048374179	1.000000(-010)	1.769062 (-006)

Table 3. The exact solution, computed solution and the error in the developed method for Problem 3.

X	Exact solution	Computed solution	Error in our method
0.100000	0.0048374180	0.004837418030	3.000000(-011)
0.200000	0.0187307531	0.01873075308	2.000000(-011)
0.300000	0.0408182207	0.04081822051	1.900000(-010)
0.400000	0.0703200460	0.07032004587	1.300000(-010)
0.500000	0.1065306597	0.1065306596	1.000000(-010)
0.600000	0.1488116361	0.1488116359	2.000000(-010)
0.700000	0.1965853038	0.1965853036	2.000000(-010)
0.800000	0.2493289641	0.2493289639	2.000000(-010)
0.900000	0.3065696597	0.3065696595	2.000000(-010)
1.000000	0.3678794412	0.3678794409	3.000000(-010)

methods derived from its first derivative and are combined to form the Three-step Optimized Block Backward Differentiation Formula (TOBBDF) on the interval from x_n to $x_{n+3} = x_n + 3h$ where h is the chosen step-length and k is the step number. We assume that the exact solution $y(x)$ on the interval $[x_n, x_{n+k}]$ is locally represented by $Y(x)$ given by (Table 2):

$$Y(x) = \sum_{j=0}^{p+q-1} b_j \phi_j(x), \tag{2}$$

b_j are unknown coefficients to be determined and $\phi_j(x)$ are polynomial basis function of degree $p+q-1$ such that the number of interpolation points p and the number of distinct collocation points q are respectively chosen to satisfy $p = k$ and $q > 0$. The proposed class of method is thus constructed by specifying the following parameters:

$$\phi_j(x) = \frac{x^{3j}}{3^j j!}, j = 0, \dots, k, p = k, q = 1, k = 3.$$

By imposing the following conditions:

$$\sum_{j=0}^6 b_j x_{n+i}^j = y_{n+i}, i = 0, \dots, \frac{5}{2}, \tag{3}$$

$$\sum_{j=0}^6 j b_j x_{n+i}^j - 1 = f_{n+i}, i = 3, \tag{4}$$

assuming that $y_{n+i} = Y(t_n + ih)$, denote the numerical approximation to the exact solution $y(x_{n+i})$, $f_{n+i} = Y'(x_n + ih, y_{n+j})$, denote the approximation to $y'(x_{n+i})$ n is the grid index (Table 3). It should be noted that Equation 3 and 4 lead to a system of seven equations that must be solved to obtain the coefficients $b_j, j = 0, 1, \dots, 6$. The main method is then obtained by substituting the values of b_j into Equation 2. After some algebraic computation, the method yields the expression in the form Equation 5:

$$Y(t) = \sum_{j=0}^{5/2} \alpha_j(t)y_{n+j} + h(\beta_3(t)f_{n+3}) \tag{5}$$

where $\alpha_j(t)$, $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}$ and $\beta_3(t)$ are continuous coefficients.

The continuous coefficients are also expressed as a function of $t = \frac{x - x_{n+2}}{h}$ given as,

$$\begin{aligned} \alpha_0(t) &= \left(\frac{4975}{1323}t^4 - \frac{1958}{2205}t^5 + \frac{548}{6615}t^6 - \frac{2351}{294}t^3 + \frac{58997}{6615}t^2 - \frac{21509}{4410}t + 1 \right) \\ \alpha_{\frac{1}{2}}(t) &= \left(-\frac{5006}{147}t^2 + \frac{5504}{147}t^3 - \frac{24}{49}t^6 + \frac{736}{147}t^5 + \frac{580}{49}t - \frac{2902}{147}t^4 \right) \\ \alpha_1(t) &= \left(\frac{2096}{49}t^4 + \frac{176}{147}t^6 + \frac{8257}{147}t^2 - \frac{710}{49}t - \frac{1712}{147}t^5 - \frac{10732}{147}t^3 \right) \\ \alpha_{\frac{3}{2}}(t) &= \left(-\frac{69196}{1323}t^2 + \frac{6256}{441}t^5 - \frac{2032}{1323}t^6 - \frac{64348}{1323}t^4 + \frac{11152}{147}t^3 + \frac{5480}{441}t \right) \\ \alpha_2(t) &= \left(-\frac{635}{98}t + \frac{52}{49}t^6 + \frac{4166}{147}t^2 + \frac{4393}{147}t^4 - \frac{12793}{294}t^3 - \frac{1366}{147}t^5 \right) \end{aligned}$$

$$\begin{aligned} \alpha_{\frac{5}{2}}(t) &= \left(\frac{1648}{147}t^3 - \frac{5198}{735}t^2 + \frac{388}{245}t - \frac{232}{735}t^6 + \frac{1936}{735}t^5 - \frac{394}{49}t^4 \right) \\ \beta_3(t) &= \left(\frac{170}{441}ht^4 + \frac{137}{441}ht^2 - \frac{10}{147}ht - \frac{20}{147}ht^5 - \frac{25}{49}ht^3 + \frac{8}{441}ht^6 \right) \end{aligned}$$

The main method is obtained for $k = 3$ by evaluating Equation 5 at $x = x_{n+3}$, which is equivalent to $t = 1$ to obtain the formula,

$$\frac{10}{49}hf_{n+3} + \frac{120}{49}y_{n+\frac{5}{2}} - \frac{150}{49}y_{n+2} + \frac{400}{147}y_{n+\frac{3}{2}} - \frac{75}{49}y_{n+1} + \frac{24}{49}y_{n+\frac{1}{2}} - \frac{10}{147}y_n = y_{n+3} \tag{6}$$

to obtain the additional methods, differentiate Equation 5 with respect to t we have,

$$Y'(t) = \frac{1}{h} \left[\sum_{j=0}^5 \bar{\alpha}_j(t)y_{n+j} + h(\bar{\beta}_3(t)f_{n+3}) \right] \tag{7}$$

Additional discrete methods are then obtained by evaluating Equation 5 at the points

$$x = [x_n, x_{n+u}, x_{n+1}, x_{n+2}], u = \frac{1}{2}, \frac{3}{2} \text{ to give:}$$

$$\begin{aligned} &-\frac{1}{4410} \frac{1}{h} \left(300hf_{n+3} + 21509y_n + 63900y_{n+1} + 28575y_{n+2} - 52200y_{n+\frac{1}{2}} - 54800y_{n+\frac{3}{2}} - 6984y_{n+\frac{5}{2}} \right) = f_n \\ &\frac{1}{882} \frac{1}{h} \left(12hf_{n+3} - 298y_n + 4320y_{n+1} + 1290y_{n+2} - 2235y_{n+\frac{1}{2}} - 2780y_{n+\frac{3}{2}} - 297y_{n+\frac{5}{2}} \right) = f_{n+\frac{1}{2}} \\ &-\frac{1}{2205} \frac{1}{h} \left(15hf_{n+3} - 152y_n + 2460y_{n+1} + 1980y_{n+2} + 1800y_{n+\frac{1}{2}} - 5680y_{n+\frac{3}{2}} - 408y_{n+\frac{5}{2}} \right) = f_{n+1} \tag{8} \\ &-\frac{1}{4410} \frac{1}{h} \left(30hf_{n+3} - 157y_n - 6840y_{n+1} + 6165y_{n+2} + 1395y_{n+\frac{1}{2}} + 400y_{n+\frac{3}{2}} - 963y_{n+\frac{5}{2}} \right) = f_{n+\frac{3}{2}} \\ &-\frac{1}{4410} \frac{1}{h} \left(60hf_{n+3} - 167y_n - 4860y_{n+1} - 6045y_{n+2} + 1320y_{n+\frac{1}{2}} + 12560y_{n+\frac{3}{2}} - 2808y_{n+\frac{5}{2}} \right) = f_{n+2} \end{aligned}$$

The methods 6, and 8 are thus combined to give the TOBBDF.

ORDER OF ACCURACY OF THE TOBBDF

The Three-step optimized block backward differentiation formulae can be represented by a matrix finite difference equation in block form as:

$$A^{(1)}Y_\omega = A^{(0)}Y_{\omega-1} + hB^{(1)}F_\omega + hB^{(0)}F_{\omega-1}, \tag{9}$$

Where:

$$\begin{aligned} Y_\omega &= \left(y_{n+\frac{1}{2}}, y_{n+1}, y_{n+\frac{3}{2}}, y_{n+2}, y_{n+\frac{5}{2}}, y_{n+3} \right)^T, Y_{\omega-1} = \left(y_{n-\frac{5}{2}}, y_{n-2}, y_{n-\frac{3}{2}}, y_{n-1}, y_{n-\frac{1}{2}}, y_n \right)^T \\ F_\omega &= \left(f_{n+\frac{1}{2}}, f_{n+1}, f_{n+\frac{3}{2}}, f_{n+2}, f_{n+\frac{5}{2}}, f_{n+3} \right)^T, F_{\omega-1} = \left(f_{n-\frac{5}{2}}, f_{n-2}, f_{n-\frac{3}{2}}, f_{n-1}, f_{n-\frac{1}{2}}, f_n \right)^T, \end{aligned}$$

for $\omega = 1, 2, \dots$ and $n = 0, 6, \dots, N - 6$.

And the matrices $A^{(1)}, A^{(0)}, B^{(1)}$ and $B^{(0)}$ are 6by 6 matrices whose entries are given by the coefficients of Equation 12 (Fotta and Alabi, 2015) given as:

$$A^{(1)} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad A^{(0)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$B^{(1)} = \begin{bmatrix} \frac{35}{72} & -\frac{487}{1920} & \frac{49}{360} & -\frac{211}{5760} & 0 & \frac{1}{640} \\ \frac{32}{45} & \frac{11}{120} & \frac{8}{135} & -\frac{7}{360} & 0 & \frac{1}{1080} \\ \frac{27}{40} & \frac{243}{640} & \frac{13}{40} & -\frac{27}{640} & 0 & \frac{1}{640} \\ \frac{32}{45} & \frac{4}{15} & \frac{32}{45} & \frac{7}{45} & 0 & 0 \\ \frac{35}{72} & \frac{325}{384} & -\frac{25}{216} & \frac{1225}{1152} & 0 & \frac{95}{3456} \\ 0 & \frac{81}{40} & -\frac{8}{5} & \frac{81}{40} & 0 & \frac{11}{40} \end{bmatrix}, \quad B^{(0)} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \frac{959}{5760} \\ 0 & 0 & 0 & 0 & 0 & \frac{169}{1080} \\ 0 & 0 & 0 & 0 & 0 & \frac{103}{640} \\ 0 & 0 & 0 & 0 & 0 & \frac{7}{45} \\ 0 & 0 & 0 & 0 & 0 & \frac{665}{3456} \\ 0 & 0 & 0 & 0 & 0 & \frac{11}{40} \end{bmatrix}$$

Following Fatunla (Abdelrahim et al., 2016) and Lambert (Rufai et al., 2016), the local truncation error associated with each of the method in the TOBBDF can be defined to be the linear difference operator:

$$L[y(t); h] = \sum_{j=0}^{k-1} \alpha_j y_{n+j} - h(\beta_{k-1} f_{n+k-1} + \beta_k f_{n+k} - \gamma_l), \quad (10)$$

where $\mathcal{A} = 1, l = 0, 1, \dots, k - 2$.

Assuming that $y(t)$ is sufficiently differentiable, we can write the terms (10) as a Taylor series expression of $y(t_{n+j})$ and $f(t_{n+j}) - y'(t_{n+j})$ as:

$$y(t_{n+j}) = \sum_{j=0}^{\infty} \frac{(jh)^m}{m!} y^{(m)}(t_n) \text{ and } y'(t_{n+j}) = \sum_{j=0}^{\infty} \frac{(jh)^{m+1}}{(m+1)!} y^{(m+1)}(t_n) \quad (11)$$

Substituting Equation 11 into Equations 10, we obtain the

expression:

$$L[y(t); h] = C_0 y(t) + C_1 h y'(t) + C_2 h^2 y''(t) + \dots + C_p h^p y^{(p)}(t) + \dots, \quad (12)$$

where the constant coefficients $C_m, m = 0, 1, 2, \dots, t = 1, 2, \dots, k$ are given as follows:

$$C_0 = \sum_{j=0}^{k-1} j \alpha_j$$

$$C_1 = \sum_{j=1}^{k-1} j \alpha_j - \beta_{k-1} - \beta_k + \gamma_l$$

$$C_2 = \frac{1}{2!} \left(\sum_{j=1}^{k-1} j^2 \alpha_j - 2(k-1)\beta_{k-1} - 2k\beta_k + 2l\gamma_l \right)$$

$$\vdots$$

$$C_m = \frac{1}{m!} \left(\sum_{j=1}^{k-1} j^m \alpha_j - m(k-1)^{m-1} \beta_{k-1} - mk^{m-1} \beta_k + ml^{m-1} \gamma_l \right)$$

where $\gamma_k = 0$ and $\gamma_l = 1, l = 0, 1, \dots, k - 2$.

The block method in Equation 9 is said to have a maximal order of accuracy m if:

$$L[y(t); h] = O(h^{m+1}), C_0 - C_1 - \dots - C_m = 0, C_{m+1} \neq 0. \quad (13)$$

Therefore, C_{m+1} is the error constant and $C_{m+1}h^{m+1}y^{(m+1)}(x_n)$ the principal local truncation error at the point x_n .

Therefore the values of the error constant calculated for the ThreestepTOBBDF (Equation 12) are given as, $(-\frac{263}{1935360}, -\frac{11}{120960}, -\frac{9}{71680}, -\frac{1}{15120}, -\frac{235}{387072}, -\frac{9}{4480})$ with order $p = (6,6,6,6,6,6)^T$ and T is the transpose.

Consistency and convergence

We note that the new block method (Equation 12) is consistent as it has order $p > 1$, since the block method (11) is zero stable. According to Bothayna and Muhammed (2019)

Convergence = zero stability + consistency.

Hence the block method (Equation 12) converges.

COMPUTING TECHNIQUE WITH THE TOBBDF

In this section, the computational techniques are presented step by step. The method is implemented more efficiently as three-step block numerical integrators for the solution of Equation 1 to simultaneously obtain the

approximations $(y_{n+\frac{1}{2}}, y_{n+1}, y_{n+\frac{3}{2}}, y_{n+2}, y_{n+\frac{5}{2}}, y_{n+3})^T$ without requiring back values and predictors, taking $n = 0, 2, \dots, N-2$, over sub-intervals $[x_0, x_3], \dots, [x_{N-2}, x_N]$, where N is the total number of

points. For instant $n = 0, w = 1, (y_{\frac{1}{2}}, y_1, y_{\frac{3}{2}}, y_2, y_{\frac{5}{2}}, y_3)^T$, are simultaneously obtained over the sub-interval $[x_0, x_3]$, as y_0 is known from Equation 1. For

$n = 1, w = 2, (y_{n+\frac{7}{2}}, y_{n+4}, y_{n+\frac{9}{2}}, y_{n+5}, y_{n+\frac{11}{2}}, y_{n+6})^T$ are simultaneously obtained over the sub-interval $[x_3, x_6]$, as y_3 is known from the previous block. Hence, the sub-

intervals do not over-lap.

Numerical examples

In this section, practical performance of the new method is examined on some test examples. We present the results obtained from the test examples which include linear, mildly stiff and highly stiff problem of initial value problems found in the literature. The results are compared with the exact solutions. The results or absolute errors $|y(x) - y_n(x)|$ are presented side by side in the table of values. All computations were carried out using Maple Mathematical Software version 17. 0, on Acer Laptop, Window 10.

Example 1

Consider the mildly stiff initial value problem (Raymond et al., 2018; Yakusat et al., 2015):

$$y' = -y, (0) = 1, h = 0.1$$

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

Example 2

Consider the highly stiff initial value problem (Raymond et al., 2018)"

$$y' = -\lambda y, (0) = 1, \lambda = 10, h = 0.1$$

$$y(x) = e^{-\lambda x}$$

Example 3

Consider the first-order stiff initial value problem (Sunday et al., 2015):

$$y' = x - y, (0) = 0, h = 0.1$$

$$y(x) = x + e^{-x} - 1$$

CONCLUSION

This work centered on the development, analysis and implementation of three-step optimized block backward differentiation formulae for the numerical solution of stiff first-order differential equations. The method was developed via backward differential formulae through the optimization of three-step. The method is consistent, convergent, zero stable and efficient for solving first-order ordinary differential equations. The results are shown in Tables 1 to 3, Tables 1 and 3 show the exact solution,

computed solution and the error while in Table 2, the comparison of error in problem 3 were made. The results perform better than Raymond (2018), which has order 8 against our method of order 6. Hence the developed method is reliable and efficient.

CONFLICT OF INTERESTS

The authors have not declared any conflict of interests.

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