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Numerical solution for stiff initial value problems using 2-point block multistep method

N Mohamad Noor¹, Z B Ibrahim¹,² and F Ismail¹,²

¹Department of Mathematics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia
²Institute for Mathematical Research, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia

E-mail: zarinabb@upm.edu.my

Abstract. This paper focuses on the derivation of an improved 2-point Block Backward Differentiation Formula of order five (I2BBDF(5)) for solving stiff first order Ordinary Differential Equations (ODEs). The I2BBDF(5) method is derived by using Taylor’s series expansion to obtain the coefficients of the formula. To verify the efficiency of the I2BBDF(5) method, stiff problems from the literature are tested and compared with the existing solver for stiff ODEs. From the numerical results, we conclude that the I2BBDF(5) method can be an alternative solver for solving stiff ODEs.

1. Introduction

Ordinary differential equations (ODEs) are widely used in various field, such as geology, economics, biology, physics and many branches of engineering as an alternative solver to approximate the solution. Many of these ODEs are known as stiff ODEs and are difficult to solve since some of the numerical methods have absolute stability restriction on the step size. Therefore, our aim in this paper is to construct an efficient multistep 2-point block method which can solved stiff ODEs efficiently.

We consider linear system of first order ODEs of the form

\[ \dot{y} = Ay + \phi(x), \quad \tilde{y}(a) = \tilde{\eta}, \quad a \leq x \leq b \]

where \( \tilde{y}^T = (y_1, y_2, \ldots, y_n) \) and \( \tilde{\eta}^T = (\eta_1, \eta_2, \ldots, \eta_r) \). Stiffness of (1) as given by Lambert [9] is as follows.

Definition 1: The linear system (1) is said to be stiff if

i. \( \text{Re}(\lambda_t) < 0, \quad t = 1, 2, \ldots, m \)

ii. \( \max_{t=1,2,\ldots,m} |\text{Re}(\lambda_t)| >> \min_{t=1,2,\ldots,m} |\text{Re}(\lambda_t)| \) where \( \lambda_t \) are the eigenvalues of \( A \). The ratio \( \frac{\max_{t=1,2,\ldots,m} |\text{Re}(\lambda_t)|}{\min_{t=1,2,\ldots,m} |\text{Re}(\lambda_t)|} \) is called the stiffness ratio.

The Backward Differentiation Formulas (BDF) which introduced by Gear [4] are well known and effective method for solving wide classes of stiff ODEs. Recently, many researchers extended the classical BDF and transform it into block methods. This extension of block methods was presented by
Ibrahim et al. [8,6,7], Yatim et al. [17], Abasi et al. [1], and Zainuddin et al. [19]. Block method can be classified into one-step method and multi-step method. Example of one-step method is the Runge-Kutta method which has been studied by Rosser [13]. Followed by Watts and Shampine [16] who studied on A-stable r-block method implicit one-step method. As for multi-step method, Voss and Abbas [15] proposed 4th order block method which are used as predictor-corrector pair for solving (1). Ibrahim et al. [5] further the research on r-point block method for solving first order ODE by developed 2-point Block Backward Differentiation Formula (2BBDF) and 3-point Block Backward Differentiation Formula (3BBDF). Nasir et al. [12] extend the idea by increasing the order of the block method which is called fifth order two-point Block Backward Differentiation Formula (BBDF(5)). Musa et al. [10] modified r-point block method to superclass block method by adding extra future points.

The method explored in this paper is closely related to the Ibrahim et al. [5] and Musa et al. [10]. The purpose of the derivation is to improve the approximation solution while compare with the existing method with same order. Formulation of the method is briefly explained in the following section. In Section 3, the stability region of the method is analyzed. The performances of the method will be present in Section 5 by solving the numerical examples in Section 4. Section 6 will discuss the numerical results obtained and a simple conclusion is made in the last section.

2. Formulation of the Method
In this section, we discussed the derivation of two-point block method using four starting values, \( y_n, y_{n-1}, y_{n-2} \) and \( y_{n-3} \) for solving (1). The method is constructed by extending the idea proposed by Musa et al. [10]. This extension is done by including extra points as backvalues in order to improve the accuracy of the solution. To construct the two-point block method, the definition of linear multi-step method (LMM) of step number \( k \) presented by Lambert [9] is used:

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

where \( \alpha_j \) and \( \beta_j \) are constant; we assume that \( \alpha_k \neq 0 \) and that not both \( \alpha_0 \) and \( \beta_0 \) are zero.

Our two-point block method is derived by represent equation (2) in the form of block multistep method, particularly with \( k = 5 \):

\[
\sum_{j=0}^{5} \alpha_{j,i} y_{n+j} = h \beta_k \left( f_{n+k} - \rho f_{n+k-1} \right) \quad i = k = 1, 2.
\]

where \( \alpha_{j,i}, \beta_k \) are the coefficients of \( y_n \) and \( f_n \) respectively. In equation (3), \( \rho \) is a free parameter that will be chosen in the interval \((−1,1)\) as stated by Vijitha-Kumara [14]. The linear difference operator \( L \) associated with equation (4) is given by

\[
L \left[ y(x_n), h \right] = \sum_{j=0}^{5} \alpha_{j,i} y_{n+j} - h \beta_k \left( f_{n+k} - \rho f_{n+k-1} \right)
\]

\[
= \alpha_{0,1} y_n + \alpha_{1,1} y_{n-1} + \alpha_{2,1} y_{n-2} + \alpha_{3,1} y_{n-3} + \alpha_{4,1} y_{n-4} + \alpha_{5,1} y_{n-5} - h \beta_k \left( f_{n+k} - \rho f_{n+k-1} \right)
\]

Expanding \( y(x_n-3h), y(x_n-2h), y(x_n-h), y(x_n), y(x_n+h), y(x_n+2h), y(x_n+kh), f(x_n+kh) \) and \( f(x_n+(k-1)h) \) using Taylor’s series and collecting like terms in \( y(x_n), y'(x_n), y''(x_n), y'''(x_n) \ldots \) yields the following
\[ L_i[y(x_n), h] = C_{0,i}y(x_n) + C_{1,i}y'(x_n) + C_{2,i}h^2y''(x_n) + C_{3,i}h^3y'''(x_n) + \ldots = 0, \quad (5) \]

where \( i = 1, 2 \). We denote the derivation for the first point as Case 1 when \( i = 1 \) and let \( \alpha_{4,1} = 1 \). Denote Case 2 (second point) when we consider \( i = 2 \) and \( \alpha_{5,2} = 1 \).

**Case 1 \((i = 1)\)**

\[
\begin{align*}
C_{0,1} &= \alpha_{0,1} + \alpha_{1,1} + \alpha_{2,1} + \alpha_{3,1} + \alpha_{5,1} = -1, \\
C_{1,1} &= -3\alpha_{0,1} - 2\alpha_{1,1} + \alpha_{2,1} + 2\alpha_{3,1} + (1 - \rho)\beta_1 = -1, \\
C_{2,1} &= \frac{9}{2}\alpha_{0,1} + 2\alpha_{1,1} + \frac{1}{2}\alpha_{2,1} + 2\alpha_{3,1} - \beta_1 = -\frac{1}{2}, \\
C_{3,1} &= -\frac{9}{2}\alpha_{0,1} - \frac{4}{3}\alpha_{1,1} - \frac{1}{6}\alpha_{2,1} + \frac{4}{3}\alpha_{3,1} - \frac{1}{2}\beta_1 = -\frac{1}{6}, \\
C_{4,1} &= \frac{27}{8}\alpha_{0,1} - \frac{2}{3}\alpha_{1,1} + \frac{1}{120}\alpha_{2,1} + \frac{2}{3}\alpha_{3,1} - \frac{1}{24}\beta_1 = -\frac{1}{24}, \\
C_{5,1} &= -\frac{81}{40}\alpha_{0,1} - \frac{4}{15}\alpha_{1,1} - \frac{1}{120}\alpha_{2,1} + \frac{4}{15}\alpha_{3,1} - \frac{1}{24}\beta_1 = -\frac{1}{120}. 
\end{align*}
\]

(6)

Using the MAPLE software, the equations in (6) are solved by choosing \( \rho = -\frac{7}{8} \) to obtain the constants of \( \alpha_{i,1} \) and \( \beta_1 \) as follows:

\[
\begin{align*}
\alpha_{0,1} &= \frac{1}{73}, \quad \alpha_{1,1} = -\frac{11}{146}, \quad \alpha_{2,1} = \frac{6}{73}, \quad \alpha_{3,1} = -\frac{82}{73}, \quad \alpha_{5,1} = \frac{15}{146}, \quad \beta_1 = \frac{48}{73}. 
\end{align*}
\]

(7)

**Case 2 \((i = 2)\)**

Similarly, we obtain the coefficients for second point as follows:

\[
\begin{align*}
\alpha_{0,2} &= -\frac{15}{236}, \quad \alpha_{1,2} = \frac{23}{59}, \quad \alpha_{2,2} = -1, \quad \alpha_{3,1} = \frac{78}{59}, \quad \alpha_{5,1} = -\frac{389}{236}, \quad \beta_2 = \frac{24}{59}. 
\end{align*}
\]

(8)

Substitute (7) and (8) into (4), we obtained the corrector formula of Improved 2-point Block Backward Differentiation Formula of order five (I2BBDF(5)) formulated as follows:

\[
\begin{align*}
y_{n+1} &= -\frac{1}{73}y_{n-3} + \frac{11}{146}y_{n-2} - \frac{6}{73}y_{n-1} + \frac{82}{73}y_n - \frac{15}{146}y_{n+2} + \frac{42}{73}h_y + \frac{48}{73}h_{f_1} + h_{f_{n+1}}, \\
y_{n+2} &= \frac{15}{236}y_{n-3} - \frac{23}{59}y_{n-2} + y_{n-1} - \frac{78}{59}y_n + \frac{389}{236}y_{n+1} + \frac{21}{59}h_{f_1} + \frac{24}{59}h_{f_{n+2}}. 
\end{align*}
\]

(9)

**3. Stability Properties of the Method**

The stability characteristic of the method is then analysed in this section. By applying scalar test equation \( y' = \lambda y, \quad \lambda < 0 \) to (9) and rearrange the formulas into matrix form will obtained the following equation
where $h\lambda = \bar{h}$ which is equivalent to $AY_m = BY_{m-1} + CY_{m-2}$. The stability polynomial of the method can be computed by using formula $R(t, \bar{h}) = \det(At^2 - Bt - C)$ where

$$A = \begin{bmatrix} 1 - \frac{48}{73} \bar{h} & 15 \frac{1}{146} \bar{h} \\ -389 & 1 - \frac{21}{236} \bar{h} \end{bmatrix}, \quad B = \begin{bmatrix} -6 \frac{73}{73} + \frac{42}{73} \bar{h} -1 \\ 1 \end{bmatrix}, \quad C = \begin{bmatrix} -1 \frac{73}{15} + \frac{11}{236} \bar{h} \\ -\frac{24}{59} \end{bmatrix}.$$ (10)

Therefore, the stability polynomial is obtained as follows.

$$R(t, \bar{h}) = \begin{vmatrix} 40291 & -8853 & -1484 \frac{t^3}{4307} & -12555 \frac{t^2}{4307} & -1152 \frac{t^1}{4307} & -19389 \frac{t^0}{8614} \\ -7443 \frac{t^4}{8614} & -416 \frac{t^3}{34456} & -19 \frac{t^2}{34456} & 882 \frac{t^1}{34456} & 315 \frac{t^0}{8614} \\ 1 & -1 \frac{21}{236} \bar{h} & 1 - \frac{24}{59} \bar{h} \\ 1 & -\frac{24}{59} \bar{h} \\ 1 & -\frac{24}{59} \bar{h} \\ 1 & -\frac{24}{59} \bar{h} \end{vmatrix}.$$ (11)

The stability region of the I2BBDF(5) method is plotted and presented in figure 1. We found that the absolute stability region covers the exterior of the circle. Hence, the method is $A$-stable since the stability region covers the entire negative half plane. (Babangida et. al [2]).

![Figure 1. Stability region of the I2BBDF(5) method.](image)

### 4. Tested Problem

To investigate the performance of I2BBDF(5) method, we apply the method on the following first order ODEs.

**Problem 1**: Linear Problem [Source: Burden and Faires [3]]

$$y' = -20y + 20 \sin x + \cos x, \quad y(0) = 1, \quad 0 \leq x \leq 2.$$

Exact solution: $y(x) = \sin x + e^{-20x}$.
Problem 2: Non-linear Problem [Source: Musa [11]]

\[ y' = \frac{50}{y} - 50y, \quad y(0) = \sqrt{2}, \quad 0 \leq x \leq 1. \]

Exact solution: \( y(x) = \sqrt{1 + e^{-100x}}. \)

Problem 3: System of 2 equations [Source: Burden and Faires [3]]

\begin{align*}
  y'_1 &= 9y_1 + 24y_2 + 5\cos x - \frac{1}{3}\sin x, \quad y_1(0) = \frac{4}{3}, \\
  y'_2 &= -24y_1 - 51y_2 - 9\cos x + \frac{1}{3}\sin x, \quad y_2(0) = \frac{2}{3}, \quad 0 \leq x \leq 10.
\end{align*}

Exact solutions: \( y_1(x) = 2e^{-3x} - e^{-39x} + \frac{1}{3}\cos x \) and \( y_2(x) = -e^{-3x} + 2e^{-39x} - \frac{1}{3}\cos x. \)

5. Numerical Results

In this section, we give some numerical examples solved by the I2BBDF(5) method and compare it with the 2-point Implicit Block Method with an Off-stage Function (2P4BBDF) method by Zainal [18] and Fifth Order Block Backward Differentiation Formula (BBDF(5)) method by Nasir et. al [12]. See [18] and [12] for the details of the algorithm. Below are the notations that will be used in the tables:

- \( h \): Step size
- \( 2P4BBDF \): 2-point Implicit Block Method with an Off-stage Function
- \( BBDF(5) \): Fifth Order Block Backward Differentiation Formula
- \( I2BBDF(5) \): Improved 2-point Block Backward Differentiation Formula of order five
- \( NS \): Number of steps taken
- \( FN \): Number of function evaluation
- \( MAXE \): Maximum Error
- \( time \): Computational time used by the method in seconds

The maximum error is evaluated by using formula

\[ MAXE = \max_{i \in \{1, \ldots, NS\}} |y_i(x) - y_i(x)| \]

where \( NS \) is the total steps, \( y_i \) is the approximate solution and \( y_i(x) \) is the analytical solution. The numerical results are shown in table 1-3.

Table 1. Numerical results for Problem 1.

| \( h \) | Method          | NS   | FN | MAXE      | time        |
|-------|----------------|------|----|-----------|-------------|
| \( 10^{-3} \) | 2P4BBDF      | 1,000| -  | 1.83398e-02 | -           |
|       | BBDF(5)       | 1,000| 3,998 | 9.71195e-04 | 3.06729e-05 |
|       | I2BBDF(5)     | 1,000| 3,997 | 7.35546e-04 | 2.87142e-06 |
| \( 10^{-5} \) | 2P4BBDF      | 100,000| - | 1.96648e-04 | -           |
|       | BBDF(5)       | 100,000| 399,998 | 1.07891e-07 | 1.41603e-03 |
|       | I2BBDF(5)     | 100,000| 400,001 | 8.01838e-08 | 1.38498e-04 |
| \( 10^{-7} \) | 2P4BBDF      | 10,000,000| - | 1.96785e-06 | -           |
|       | BBDF(5)       | 10,000,000| 39,999,998 | 3.35482e-11 | 2.27564e-02 |
|       | I2BBDF(5)     | 10,000,000| 40,000,001 | 2.81187e-11 | 1.34132e-02 |
Table 2. Numerical results for Problem 2.

| $h$   | Method   | NS     | FN     | MAXE          | time            |
|-------|----------|--------|--------|---------------|-----------------|
| $10^{-3}$ | 2P4BBDF  | 500    | -      | 2.824e-02    | -               |
|       | BBDF(5)  | 500    | 1,998  | 4.88893e-03  | 5.61089e-06     |
|       | I2BBDF(5)| 500    | 1,997  | 3.89820e-03  | 1.99995e-06     |
| $10^{-5}$ | 2P4BBDF  | 50,000 | -      | 3.6525e-04   | -               |
|       | BBDF(5)  | 50,000 | 199,998| 7.13439e-07  | 2.21668e-04     |
|       | I2BBDF(5)| 50,000 | 199,997| 5.30439e-07  | 4.12432e-05     |
| $10^{-7}$ | 2P4BBDF  | 5,000,000 | -  | 3.66172e-06  | -               |
|       | BBDF(5)  | 5,000,000 | 19,999,998  | 7.15947e-11  | 1.00759e-02     |
|       | I2BBDF(5)| 5,000,000 | 19,999,997  | 5.31992e-11  | 5.61090e-03     |

Table 3. Numerical results for Problem 3.

| $h$   | Method    | NS     |FN     | MAXE           | time            |
|-------|-----------|--------|--------|----------------|-----------------|
| $10^{-3}$ | 2P4BBDF  | 5,000  | -      | 6.77482e-02   | -               |
|       | BBDF(5)   | 5,000  | 39,998 | 6.64841e-03   | 7.73547e-05     |
|       | I2BBDF(5) | 5,000  | 39,997 | 5.12864e-03   | 3.62559e-05     |
| $10^{-5}$ | 2P4BBDF  | 500,000 | -    | 7.75727e-04   | -               |
|       | BBDF(5)   | 500,000 | 3,999,998 | 8.17344e-07  | 3.79007e-03     |
|       | I2BBDF(5) | 500,000 | 3,999,997  | 6.07555e-07  | 2.12218e-03     |
| $10^{-7}$ | 2P4BBDF  | 50,000,000 | -    | 7.76778e-06   | -               |
|       | BBDF(5)   | 50,000,000 | 399,999,998 | 1.59108e-10  | 9.90200e-01     |
|       | I2BBDF(5) | 50,000,000 | 400,000,005 | 1.25315e-10  | 2.89056e-01     |

The errors generated by the methods are depicted in Figure 1-3.

Figure 2. Efficiency curves for Problem 1.
6. Discussion

In this section the performance of 2P4BBDF, BBDF(5) and I2BBDF(5) methods are discussed in terms of its accuracy, number of function evaluations and computational time. We choose 2P4BBDF and BBDF(5) as the method of comparison since the method is of the same order as the derived method. Table 1, 2 and 3 presents the numerical results obtained from 2P4BBDF, BBDF(5) and I2BBDF(5) methods. Based on table 1-3, the maximum error is getting smaller as the \( h \) decreases. As for 2P4BBDF method, we only compare in terms of the accuracy since the code is not available to run for computational time and function evaluation. Meanwhile, figure 1, 2 and 3 shows the efficiency of the method in terms of maximum error versus number of function evaluation as well as the maximum error versus computation time required by BBDF(5) and I2BBDF(5) methods. From the graphs of log MAXE against log FN, its show that the I2BBDF(5) method gives better performance compared to the
BBDF(5) method. In terms of the computational time, the maximum error decreased as execution time increased. Therefore, the I2BBDF(5) method is more efficient as compare to the BBDF(5) method.

7. Conclusion
In this paper, we have discussed the derivation of an Improved 2-point Block Backward Differentiation Formula of order five, (I2BBDF(5)) method for solving first order stiff ODEs. These new I2BBDF(5) method enhanced the accuracy of the numerical solutions and reduced computational time. Further research into variation of stepsize for the solution of ODEs will be useful to increase the efficiency further.

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