PAPER • OPEN ACCESS

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

IOP ebooks™

Bringing you innovative digital publishing with leading voices to create your essential collection of books in STEM research.

Start exploring the collection - download the first chapter of every title for free.

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

N Mohamad Noor[1], Z B Ibrahim[1,2] and F Ismail[1,2]

[1]Department of Mathematics, Faculty of Science, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, Malaysia
[2]Institute 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

$$\tilde{y}' = A\tilde{y} + \tilde{\phi}(x), \quad \tilde{y}(a) = \tilde{\eta}, \quad a \le x \le b \tag{1}$$

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

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

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

ii. $\displaystyle\max_{t=1,2,\ldots,m} |\operatorname{Re}(\lambda_t)| \gg \min_{t=1,2,\ldots,m} |\operatorname{Re}(\lambda_t)|$ where λ_t are the eigenvalues of A. The ratio $\dfrac{\max\limits_{t=1,2,\ldots,m} |\operatorname{Re}(\lambda_t)|}{\min\limits_{t=1,2,\ldots,m} |\operatorname{Re}(\lambda_t)|}$ 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:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}, \tag{2}$$

where α_j and β_j are constant; we assume that $\alpha_k \neq 0$ and that not both α_0 and β_0 are zero.

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

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

where $\alpha_{j,i}$, β_k are the coefficients of y_n and f_n respectively. In equation (3), ρ 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

$$L_i[y(x_n), h] = \sum_{j=0}^{5} \alpha_{j,i} y_{n+j-3} - h\beta_k \left(f_{n+k} - \rho f_{n+k-1} \right)$$

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

$$= \alpha_{0,i} y(x_n - 3h) + \alpha_{1,i} y(x_n - 2h) + \alpha_{2,i} y(x_n - h) + \alpha_{3,i} y(x_n) + \alpha_{4,i} y(x_n + h)$$

$$+ \alpha_{5,i} y(x_n + 2h) - h\beta_k \left(f(x_n + kh) - \rho f(x_n + (k-1)h) \right).$$

Expanding $y(x_n - 3h)$, $y(x_n - 2h)$, $y(x_n - h)$, $y(x_n)$, $y(x_n + h)$, $y(x_n + 2h)$, $f(x_n + kh)$ and $f(x_n + (k-1)h)$ using Taylor's series and collecting like terms in $y(x_n)$, $y'(x_n)$, $y''(x_n)$, $y'''(x_n)$,... yields the following

$$L_i[y(x_n), h] = C_{0,i}\, y(x_n) + C_{1,i}\, hy'(x_n) + C_{2,i}\, h^2 y''(x_n) + C_{3,i}\, h^3 y'''(x_n) + \ldots = 0, \tag{5}$$

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 ($i = 1$)

$$C_{0,1} = \alpha_{0,1} + \alpha_{1,1} + \alpha_{2,1} + \alpha_{3,1} + \alpha_{5,1} = -1,$$

$$C_{1,1} = -3\alpha_{0,1} - 2\alpha_{1,1} - \alpha_{2,1} + 2\alpha_{5,1} - (1 - \rho)\beta_1 = -1,$$

$$C_{2,1} = \frac{9}{2}\alpha_{0,1} + 2\alpha_{1,1} + \frac{1}{2}\alpha_{2,1} + 2\alpha_{5,1} - \beta_1 = -\frac{1}{2},$$

$$C_{3,1} = -\frac{9}{2}\alpha_{0,1} - \frac{4}{3}\alpha_{1,1} - \frac{1}{6}\alpha_{2,1} + \frac{4}{3}\alpha_{5,1} - \frac{1}{2}\beta_1 = -\frac{1}{6}, \tag{6}$$

$$C_{4,1} = \frac{27}{8}\alpha_{0,1} + \frac{2}{3}\alpha_{1,1} + \frac{1}{24}\alpha_{2,1} + \frac{2}{3}\alpha_{5,1} - \frac{1}{6}\beta_1 = -\frac{1}{24},$$

$$C_{5,1} = -\frac{81}{40}\alpha_{0,1} - \frac{4}{15}\alpha_{1,1} - \frac{1}{120}\alpha_{2,1} + \frac{4}{15}\alpha_{5,1} - \frac{1}{24}\beta_1 = -\frac{1}{120}.$$

Using the MAPLE software, the equations in (6) are solved by choosing $\rho = -\dfrac{7}{8}$ to obtain the constants of $\alpha_{j,1}$ and β_1 as follows:

$$\alpha_{0,1} = \frac{1}{73}, \quad \alpha_{1,1} = -\frac{11}{146}, \quad \alpha_{2,1} = \frac{6}{73}, \quad \alpha_{3,1} = -\frac{82}{73}, \quad \alpha_{5,1} = \frac{15}{146}, \quad \beta_1 = \frac{48}{73}. \tag{7}$$

Case 2 ($i = 2$)
Similarly, we obtain the coefficients for second point as follows:

$$\alpha_{0,2} = -\frac{15}{236}, \quad \alpha_{1,2} = \frac{23}{59}, \quad \alpha_{2,2} = -1, \quad \alpha_{3,1} = \frac{78}{59}, \quad \alpha_{5,1} = -\frac{389}{236}, \quad \beta_2 = \frac{24}{59}. \tag{8}$$

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:

$$y_{n+1} = -\frac{1}{73}y_{n-3} + \frac{11}{146}y_{n-2} - \frac{6}{73}y_{n-1} + \frac{82}{73}y_n - \frac{15}{146}y_{n+2} + \frac{42}{73}hf_n + \frac{48}{73}hf_{n+1},$$

$$y_{n+2} = \frac{15}{236}y_{n-3} - \frac{23}{59}y_{n-2} + y_{n-1} - \frac{78}{59}y_n + \frac{389}{236}y_{n+1} + \frac{21}{59}hf_{n+1} + \frac{24}{59}hf_{n+2}. \tag{9}$$

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

$$\begin{bmatrix} 1-\dfrac{48}{73}\overline{h} & \dfrac{15}{146} \\ -\dfrac{389}{236}-\dfrac{21}{59}\overline{h} & 1-\dfrac{24}{59}\overline{h} \end{bmatrix}\begin{bmatrix} y_{n+1} \\ y_{n+2} \end{bmatrix} = \begin{bmatrix} -\dfrac{6}{73} & \dfrac{82}{73}+\dfrac{42}{73}\overline{h} \\ 1 & -\dfrac{78}{59} \end{bmatrix}\begin{bmatrix} y_{n-1} \\ y_n \end{bmatrix} + \begin{bmatrix} -\dfrac{1}{73} & \dfrac{11}{146} \\ \dfrac{15}{236} & -\dfrac{23}{59} \end{bmatrix}\begin{bmatrix} y_{n-3} \\ y_{n-2} \end{bmatrix} \qquad (10)$$

where $h\lambda = \overline{h}$ which is equivalent to $AY_m = BY_{m-1} + CY_{m-2}$. The stability polynomial of the method can be compute by using formula $R(t,\overline{h}) = \det[At^2 - Bt - C]$ where

$$A = \begin{bmatrix} 1-\dfrac{48}{73}\overline{h} & \dfrac{15}{146} \\ -\dfrac{389}{236}-\dfrac{21}{59}\overline{h} & 1-\dfrac{24}{59}\overline{h} \end{bmatrix}, \quad B = \begin{bmatrix} -\dfrac{6}{73} & \dfrac{82}{73}+\dfrac{42}{73}\overline{h} \\ 1 & -\dfrac{78}{59} \end{bmatrix}, \quad C = \begin{bmatrix} -\dfrac{1}{73} & \dfrac{11}{146} \\ \dfrac{15}{236} & -\dfrac{23}{59} \end{bmatrix}.$$

Therefore, the stability polynomial is obtained as follows.

$$\begin{aligned} R(t,\overline{h}) = {}& \frac{40291}{34456}t^4 - \frac{8853}{8614}t^4\overline{h} - \frac{1484}{4307}t^3 - \frac{12555}{17228}t^2 + \frac{1152}{4307}t^4\overline{h}^2 - \frac{19389}{8614}t^3\overline{h} \\ & - \frac{7443}{8614}t^2\overline{h} - \frac{416}{4307}t + \frac{19}{34456} - \frac{882}{4307}t^3\overline{h}^2 - \frac{315}{8614}t\overline{h} \end{aligned} \qquad (11)$$

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]).
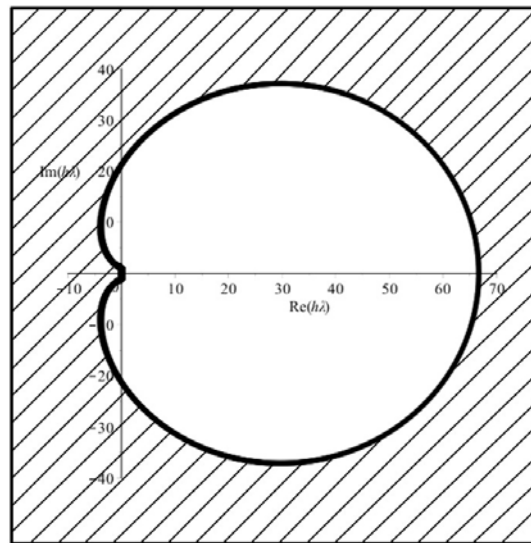

Figure 1. Stability region of the I2BBDF(5) method.

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]]

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

Exact solution: $y(x) = \sin x + e^{-20x}$.

Problem 2: Non-linear Problem [Source: Musa [11]]

$$y' = \frac{50}{y} - 50y, \quad y(0) = \sqrt{2}, \quad 0 \le x \le 1.$$

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

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

$$y_1' = 9y_1 + 24y_2 + 5\cos x - \frac{1}{3}\sin x, \quad y_1(0) = \frac{4}{3},$$

$$y_2' = -24y_1 - 51y_2 - 9\cos x + \frac{1}{3}\sin x, \quad y_2(0) = \frac{2}{3}, \quad 0 \le x \le 10.$$

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

$$MAXE = \max_{1 \le t \le NS} \left| (y_i)_t - (y(x_i))_t \right|$$

where *NS* is the total steps, y_i is the approximate solution and $y(x_i)$ 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
	2P4BBDF	1,000	-	1.83398e-02	-
10^{-3}	BBDF(5)	1,000	3,998	9.71195e-04	3.06729e-05
	I2BBDF(5)	1,000	3,997	7.35546e-04	2.87142e-06
	2P4BBDF	100,000	-	1.96648e-04	-
10^{-5}	BBDF(5)	100,000	399,998	1.07891e-07	1.41603e-03
	I2BBDF(5)	100,000	400,001	8.01838e-08	1.38498e-04
	2P4BBDF	10,000,000	-	1.96785e-06	-
10^{-7}	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	-	2.82446e-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	-	3.65253e-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.
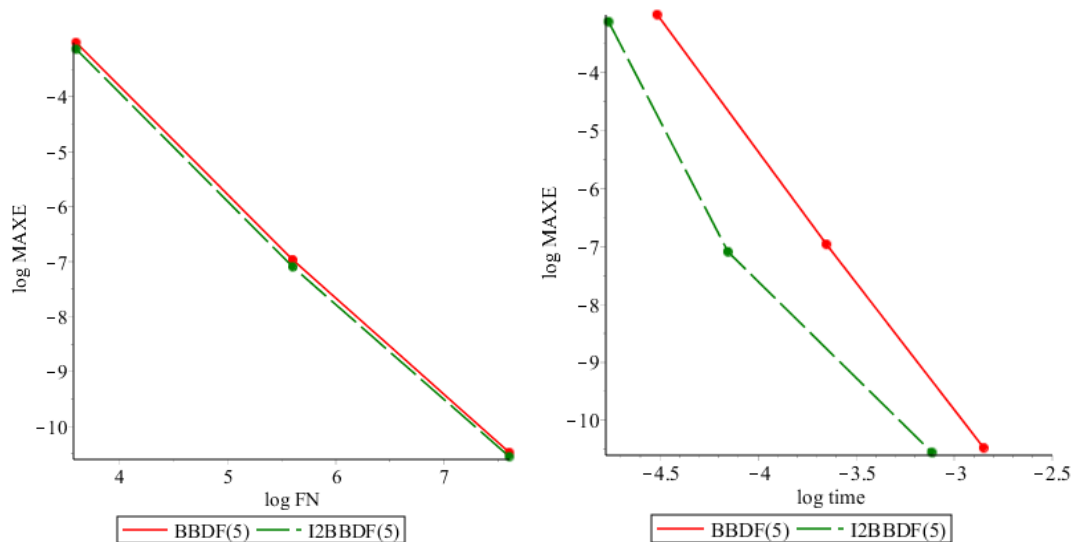
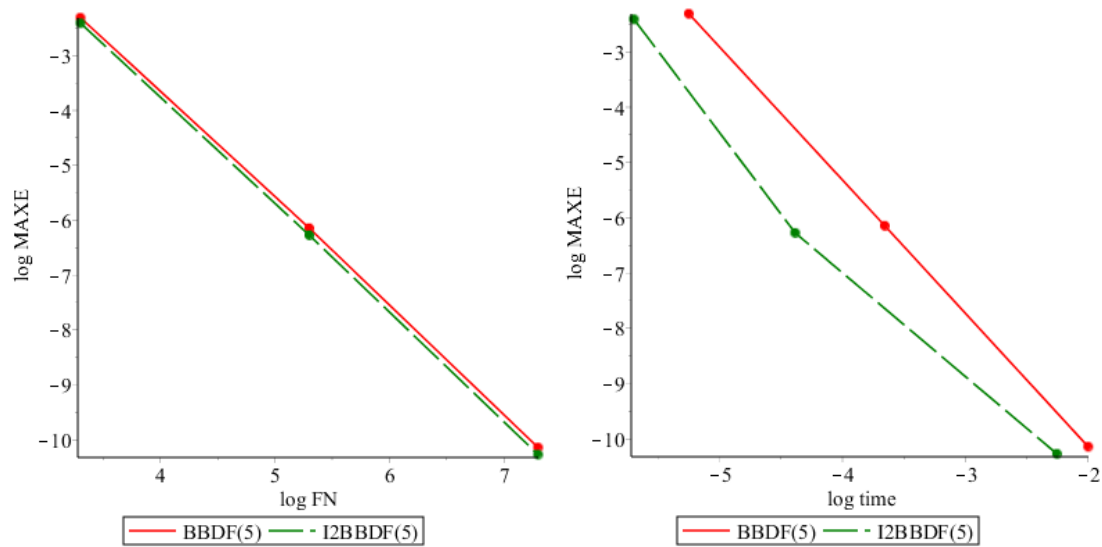**Figure 2.** Efficiency curves for Problem 1.
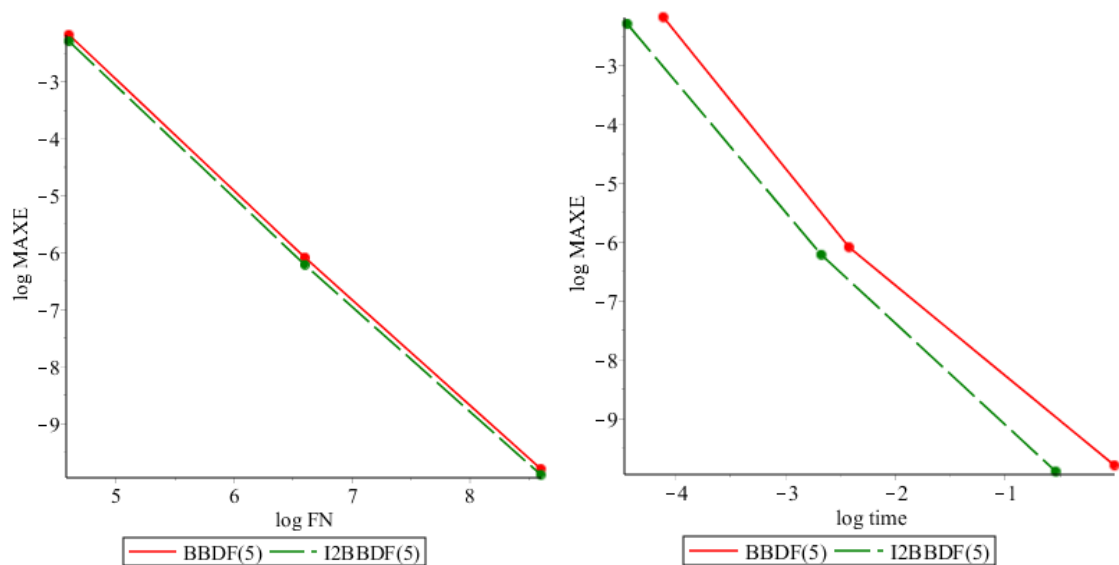
Figure 3. Efficiency curves for Problem 2.

Figure 4. Efficiency curves for Problem 3.

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.

Acknowledgement

References

[1] Abasi N, Suleiman M, Abbasi N and Musa H 2014 2-point Block BDF Method with Off-step Points for Solving Stiff ODEs *Journal of Soft Computing and Applications* **2014** 1-15
[2] Babangida B, Musa H and Ibrahim L K 2016 A New Numerical Method for Solving Stiff Initial Value Problems *Fluid Mechanics: Open Access* **3** 1-5
[3] Burden R L and Faires J D 2001 Numerical Analysis, PWS-KENT Publishing Company, Boston, Seventh edition
[4] Gear C W 1971 *Numerical Initial Value Problems in Ordinary Differential Equations* (New Jersey: Prentice Hall, Inc)
[5] Ibrahim Z B, Othman K I and Suleiman M 2007(a) Implicit *r*-point Block Backward Differentiation Formula for Solving First-Order Stiff ODEs *Applied Mathematics and Computation.* **186** 558-565
[6] Ibrahim Z B, Othman K I and Suleiman M 2007(b) Variable Step Block Bacward Differentiation Formula for Solving First Order Stiff ODEs *Proceedings of the World Congress in Engineering.* **2** 785-789
[7] Ibrahim Z B, Suleiman M and Othman K I 2008 Direct Block Backward Differentiation Formulas for Solving Second Order Ordinary Differential Equations *International Journal of Mathematical, Computational, Physical, Electrical and Computer Engineering.* **2** 260-262
[8] Ibrahim Z B, Suleiman M and Othman K I 2008 Fixed Coefficients Block Backward Differentiation Formulas for the Numerical Solution of Stiff Ordinary Differential Equations *European Journal of Scientific Research.* **21** 508-520
[9] Lambert J D, 1973 *Computational Methods in Ordinary Differential Equations* (New York: John Wiley and Sons)
[10] Musa H, Suleiman M B, Ismail F, Senu N and Ibrahim Z B 2013 An Improved 2-point Block Backward Differentiation Formula for Solving Stiff Initial Value Problems *AIP Conf. Proc.* **1522** 211-220
[11] Musa H 2013 *New Classes of Block Backward Differentiation Formula for Solving Stiff Initial Value Problems* PhD Thesis, UPM
[12] Nasir N A A M, Ibrahim Z B, Othman K I and Suleiman M 2012 Numerical Solution of First Order Stiff Ordinary Differential Equations using Fifth Order Block Backward Differentiation Formulas *Sains Malaysiana* **41** 489-492
[13] Rosser J B 1967 A Runge-Kutta for All Seasons *SIAM* **9** 417-440
[14] Vijitha-Kumara K H Y 1985 *Variable Stepsize Variable Order Multistep Methods for Stiff Ordinary Differential Equations* PhD Thesis, Iowa States University
[15] Voss D and Abbas S 1997 Block Predictor-Corrector Schemes for the Parallel Solution of ODEs *Comp. Math. Applic.* **33** 65-72

[16] Watts H A and Shampine L F 1972 *A*-stable Block Implicit One-Step Methods *BIT.* **12** 252-266

[17] Yatim S A M, Ibrahim Z B, Othman K I and Suleiman M B 2013 A Numerical Algorithm for Solving Stiff Ordinary Differential Equations *Mathematical Problems in Engineering.* **2013** Article ID 989381

[18] Zainal S Z 2014 *Fifth Order 2-point Implicit Block Method with and Off-stage Function for Solving First Order Stiff Initial Value Problems* Master Thesis, UPM

[19] Zainuddin N, Ibrahim Z B, Othman K I and Suleiman M 2016 Direct Fifth Order Block Backward Differentiation Formulas for Solving Second Order Ordinary Differential Equations *Chiang Mai J. Sci.* **43** 1171-1181