Numerical Solver of A(alpha)-stable for Stiff Ordinary Differential Equations

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***Abstract*— In this paper, a numerical solver for stiff ordinary differential equations (ODEs) known as the Extended Singly Diagonally Implicit Block Backward Differentiation Formulas (ESDIBDDF) is developed. Objectives of this study are to analyse the $A(\alpha)-$ stability of the ESDIBBDF method and enhance its accuracy by employing a strategy that minimizes the error norm to optimize the values of free parameters. In addition to that, accuracy of the method is to be enhanced by approximating solutions by implementing extra functions to be evaluated. The formula is specifically designed in a lower triangular form with equal diagonal coefficients, enabling faster computation of numerical solutions. Numerical experiments are conducted to assess the efficiency of this method as a solver for stiff ODEs, comparing it with existing methods. The $A(\alpha)-$ stability analysis is verified and conditions for convergence are discussed. The conclusive works efficiently as an alternate solver for stiff ODEs. The research recommended extended application of the developed method to solve applied problems.**

***Index Terms*— singly diagonally implicit, block multistep method, $A(\alpha)-$ stable, stiff ODEs**

I. Introduction

NUMEROUS physical systems give rise to equations that are expressed in terms of unknown quantities, with their derivatives being referred to as differential equations (DEs). When these derivatives are taken with respect to a single independent variable, the system is classified as ordinary differential equations (ODEs), and the magnitudes of their eigenvalues can vary significantly. Many of these systems exhibit a challenging characteristic known as stiffness. This phenomenon is encountered in various applications such as the analysis of biological sciences, mechanical systems, diffusion, electric circuits, and chemical kinetics. The focus of this research is on investigating a linear system of first-order stiff ODEs, represented by the form

$$y'(x) = f(x,y), \quad y(a)=\eta, \quad x\in[a,b], \tag{1}$$

where $y^T=(y_1,y_2,\ldots,y_m)$, $f^T=(f_1,f_2,\ldots,f_m)$ and $\eta^T=(\eta_1,\eta_2,\ldots,\eta_m)$. Equation (1) satisfies the condition of linearity if $f(x,y)=A(x)y+\phi(x)$ where $A(x)$ is a constant $m\times m$ matrix and $\phi(x)$ is an $m-$dimensional vector.

In order to ensure the reliability of the predicted solutions for the given differential equations and their initial conditions, it is necessary to establish the existence and uniqueness of the solution, which can be achieved by verifying the satisfaction of the Lipschitz condition, as stated in the following theorem.

Theorem 1. *Let $f(x,y(x))$ defined and continuous for all points $(x,y(x))$ in a domain D defined by $a\le x\le b$, $y\in(-\infty,\infty)$, a and b are finite, and that $f(x,y(x))$ satisfies Lipschitz condition. Then for any given number μ, there exists a unique solution $y(x)$ of (1), where for all $(x,y(x))\in D$, $y(x)$ is continuous and differentiable.*

Throughout the centuries, the scientific literature has presented numerous concepts and understandings of stiffness. Based on the research by [1], the following definition of stiffness should be considered for the development of the proposed solver.

Definition 1. *Linear system (1) is said to be stiff if*

i. $\mathrm{Re}(\lambda_i)<0$, $i=1,2,\ldots,m$ *and*

ii. $\max_i|\mathrm{Re}(\lambda_i)|>>\min_i|\mathrm{Re}(\lambda_i)|$, *where* λ_i *are the eigenvalues of* A *and the ratio* $S=\max_i|\mathrm{Re}(\lambda_i)|\big/\min_i|\mathrm{Re}(\lambda_i)|$ *is called the stiffness ratio.*

Due to the limitations of analytical methods in accurately computing solutions for most differential equations, the utilization of numerical methods becomes necessary. Numerical methods for approximating solutions of ODEs are commonly classified into two categories: one-step methods, such as Euler and Runge-Kutta (RK) methods, and multistep methods, including backward differentiation formulas (BDF) and Adams method. The objective of this study is to introduce a novel extended numerical hybrid-like formula, referred to as Extended Singly Diagonally Implicit Block Backward Differentiation Formulas (ESDIBDDF). The development of this method considers both one-step

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and multistep methods, while addressing the stability behavior associated with stiffness. Among the active research related to the idea are elaborated in [2] and [3] which show different approaches in "hybriding" methods from two different backgrounds. Meanwhile, studies on the $A(\alpha)-$stability properties of numerical methods, specifically the RK methods, by [4] show that those methods are able to solve problems of stiffness efficiently.

The Singly Diagonally Implicit RK (SDIRK) was first proposed by [5] which emphasized the requirement of identical diagonal coefficients, $a_{ii}=\gamma$. This condition ensures that the linear system, when solved using Newton iteration, adopts the form of $I-h\alpha J$. As a result, the computational cost of predicting solutions is reduced, as the system is solved with the same matrix for each time step, as mentioned in [6]. Besides, the singly diagonally implicit approach overcomes certain limitations encountered by both fully implicit and explicit RK methods, as discussed in [7].

In [8], the Block BDF (BBDF) method demonstrated better performance compared to the classical BDF method in solving stiff problems, achieving improved accuracy and execution time. Instead of estimating solutions individually, the method employs a block-wise approach by utilizing the previous block of backvalues. To enhance the accuracy of the BBDF method, [9] introduced the Block Extended BDF (BEBDF) method, which includes additional function evaluations.

The relevance of a method in solving stiff problems is demonstrated by its stability properties. According to [10], the proposed method must be at least almost $A-$stable to solve stiff problems. Meanwhile, [11] introduced a method with $L(\alpha)-$stability which is the requirement for numerical integration for stiff initial value problems. The Singly Diagonally Implicit BBDF (SDIBBDF) method developed in [3], offers enhanced $A-$stability and effectively estimates solutions for stiff problems compared to other existing solvers. Additionally, [12] introduces the $A(\alpha)$ Stable BBDF with fixed coefficients, emphasizing its ability to efficiently solve stiff ODEs while maintaining stability.

Furthermore, this research will examine the error norm minimization technique proposed by [13] to attain a specific order of accuracy. This technique involves selecting free parameters of the principal error norm of the method, as expressed by the following equation.

$$A^{(p+1)}=\|\tau^{(p+1)}\|_2=\sqrt{\sum_{j=1}^{n_{p+1}}\tau^{(p+1_j)^2}} \tag{2}$$

Therefore, the objective is to develop the $A(\alpha)-$ESDIBDDF method that is capable to solve stiff ODEs efficiently.

The structure of the paper is as follows: The subsequent section provides the derivation of the proposed method, while the following sections focus on the analysis of convergence and stability. Section V delves into the implementation of the method, while Section VI discusses the numerical simulations conducted. Finally, the overall findings of the research are concluded in Section VII.

II. Research Methodology

First, the general linear multistep method (LMM) for first-order ODEs is examined in the following manner.

$$\sum_{j=0}^{k}\alpha_j y_{n+j}=h\sum_{j=0}^{k}\beta_j y'_{n+j}, \tag{3}$$

where α_j and β_j are constants by assuming that not both α_0 and β_0 are zero, with $\alpha_k\neq 0$. k is the order of the method and h is the step size.

Subsequently, the linear difference operator is formulated for the $A(\alpha)-$Extended Singly Diagonally Implicit BBDF ($A(\alpha)-$ESDIBBDF) method, incorporating additional function evaluation, as demonstrated below.

$$L_s(y(x);h):\sum_{j=0}^{k+s-1}\alpha_{s,j-2}y_{n+j-2}=h\sum_{j=3}^{k+s-1}\beta_{s,k+j-2}f_{n+j-2} \tag{4}$$

where $k=3$; $s=1,2,3$ for y_{n+1}, y_{n+2} and y_{n+3} respectively.

In order to establish a singly diagonally implicit behavior, the diagonal elements of the method are set as $\alpha_{i,i}=\gamma$ and $\beta_{i,i}=\beta$. Then, we expand (4) to get

$$\begin{aligned}L_1(y(x);h)&=\alpha_{1,-2}y_{n-2}+\alpha_{1,-1}y_{n-1}+\alpha_{1,0}y_n+\gamma y_{n+1}-h\beta f_{n+1}\\ L_2(y(x);h)&=\alpha_{2,-2}y_{n-2}+\alpha_{2,-1}y_{n-1}+\alpha_{2,0}y_n+\alpha_{2,1}y_{n+1}+\\&\quad\gamma y_{n+2}-h\left(\beta_{2,4}f_{n+1}+\beta f_{n+2}\right)\\ L_3(y(x);h)&=\alpha_{3,-2}y_{n-2}+\alpha_{3,-1}y_{n-1}+\alpha_{3,0}y_n+\alpha_{3,1}y_{n+1}+\\&\quad\alpha_{3,2}y_{n+2}+\gamma y_{n+3}-h\left(\beta_{3,4}f_{n+1}+\beta_{3,5}f_{n+2}+\beta f_{n+3}\right)\end{aligned} \tag{5}$$

Equation (5) is arranged in matrix form, and each column matrix is let as A_j and B_j as follows:

$$\overset{A_0\quad A_1\quad A_2}{\begin{bmatrix}\alpha_{1,-2}&\alpha_{1,-1}&\alpha_{1,0}\\ \alpha_{2,-2}&\alpha_{2,-1}&\alpha_{2,0}\\ \alpha_{3,-2}&\alpha_{3,-1}&\alpha_{3,0}\end{bmatrix}}\begin{bmatrix}y_{n-2}\\ y_{n-1}\\ y_n\end{bmatrix}+\overset{A_3\quad A_4\quad A_5}{\begin{bmatrix}\gamma&0&0\\ \alpha_{2,1}&\gamma&0\\ \alpha_{3,1}&\alpha_{3,2}&\gamma\end{bmatrix}}\begin{bmatrix}y_{n+1}\\ y_{n+2}\\ y_{n+3}\end{bmatrix}= h\overset{B_3\quad B_4\quad B_5}{\begin{bmatrix}\beta&0&0\\ \beta_{2,4}&\beta&0\\ \beta_{3,4}&\beta_{3,5}&\beta\end{bmatrix}}\begin{bmatrix}f_{n+1}\\ f_{n+2}\\ f_{n+3}\end{bmatrix} \tag{6}$$

Taylor series expansion about $x=x_n$ is applied to the approximate relations of (5), and the y' terms are collected which yields

$$L_s(y(x);h)=C_0y(x)+C_1y'(x)+\ldots+C_qy^q(x)+\ldots, \tag{7}$$

where

$$C_0 = \sum_{j=0}^{k+2} A_j,$$
$$C_1 = \sum_{j=0}^{k+2} jA_j - \sum_{j=0}^{w} B_j, \quad (8)$$
$$C_q = \frac{1}{q!}\sum_{j=0}^{5} j^q A_j - \frac{1}{(q-1)!}\sum_{j=3}^{5} j^{q-1} B_j, \qquad q = 2,3,\ldots.$$

Equation (8) is expanded up to $q = 3$ to develop a third order method. The corresponding C_0, C_1, C_2 and C_3 will result in 12 variables and 5 free parameters. By $C_0 = C_1 = C_2 = C_3 = 0$ simultaneously in terms of free parameters, we get

$$\alpha_{1,-2} = -\frac{1}{3}\beta, \quad \alpha_{1,-1} = \frac{3}{2}\beta, \quad \alpha_{1,0} = -3\beta, \quad \alpha_{2,-2} = -\frac{1}{3}\beta_{2,3},$$
$$\alpha_{2,-1} = \frac{3}{2}\beta_{2,3} - \frac{1}{3}\beta, \quad \alpha_{2,0} = -3\beta_{2,3} + \frac{3}{2}\beta,$$
$$\alpha_{2,1} = \frac{11}{6}\beta_{2,3} - 3\beta, \quad \alpha_{3,-2} = -\frac{1}{4}\alpha_{3,1} + \frac{1}{8}\beta_{3,3} - \frac{3}{4}\beta_{3,4} + \frac{3}{8}\beta,$$
$$\alpha_{3,-1} = \alpha_{3,1} - \frac{1}{3}\beta_{3,3} + \frac{8}{3}\beta_{3,4} - \frac{3}{2}\beta,$$
$$\alpha_{3,0} = -\frac{3}{2}\alpha_{3,1} - \frac{1}{4}\beta_{3,3} - 3\beta_{3,4} + \frac{23}{12}\beta,$$
$$\alpha_{3,2} = -\frac{1}{4}\alpha_{3,1} + \frac{11}{24}\beta_{3,3} + \frac{13}{12}\beta_{3,4} - \frac{21}{8}\beta, \quad \gamma = \frac{11}{6}\beta. \quad (9)$$

The error condition of the $A(\alpha)-$ESDIBBDF method is considered as

$$C_4 = \begin{bmatrix} -\frac{1}{4}\beta \\ -\frac{1}{4}\beta_{2,3} - \frac{1}{4}\beta \\ -\frac{1}{4}\alpha_{3,1} + \frac{5}{24}\beta_{3,3} - \beta_{3,4} + \frac{1}{8}\beta \end{bmatrix}.$$

By implementing the strategy of minimizing the error norm as discussed in [9], through elimination technique, we choose $\beta = \frac{1}{10}$, $\beta_{2,3} = \beta_{3,3} = \beta_{3,4} = \frac{1}{100}$ and $\alpha_{3,1} = -\frac{3}{40}$. Thus, the principal error norm (2) of the proposed method is $A^{(4)} = 0.23936$.

The free parameters chosen are then substituted into (9) to get the following coefficients.

$$\alpha_{1,-2} = -\frac{1}{30}, \quad \alpha_{1,-1} = \frac{3}{20}, \quad \alpha_{1,0} = -\frac{3}{10}, \quad \alpha_{2,-2} = -\frac{1}{300},$$
$$\alpha_{2,-1} = -\frac{11}{600}, \quad \alpha_{2,0} = \frac{3}{25}, \quad \alpha_{2,1} = -\frac{169}{600}, \quad \alpha_{3,-2} = \frac{1}{20},$$
$$\alpha_{3,-1} = -\frac{121}{600}, \ \alpha_{3,0} = \frac{163}{600}, \ \alpha_{3,2} = -\frac{137}{600}, \ \gamma = \frac{11}{60}.$$

The values obtained are then substituted into (5), and by rearranging the equations, the following general corrector formula of $A(\alpha)-$ESDIBBDF method is obtained.

$$y_{n+1} = \frac{2}{11}y_{n-2} - \frac{9}{11}y_{n-1} + \frac{18}{11}y_n + \frac{6}{11}hf_{n+1}^{(p)},$$
$$y_{n+2} = \frac{1}{55}y_{n-2} + \frac{1}{10}y_{n-1} - \frac{36}{55}y_n + \frac{169}{110}y_{n+1} + \frac{3}{55}hf_{n+1}^{(p)} + \frac{6}{11}hf_{n+2}^{(p)},$$
$$y_{n+3} = -\frac{3}{11}y_{n-2} + \frac{11}{10}y_{n-1} - \frac{163}{110}y_n + \frac{9}{2}y_{n+1} + \frac{137}{110}y_{n+2} + \frac{3}{55}hf_{n+1}^{(p)} + \frac{3}{55}hf_{n+2}^{(p)} + \frac{6}{11}hf_{n+3}^{(p)}. \quad (10)$$

Since the $A(\alpha)-$ESDIBBDF method is of implicit nature, an explicit method, is necessary to estimate the solutions, denoted as y_{n+s}, for the corrector. The predicted value serves as an initial approximation for $y_{n+s}^{(0)}$. To derive the predictor formula for the method, Lagrange interpolation is employed to obtain

$$y_{n+1}^{(p)} = 4y_n - 6y_{n-1} + 4y_{n-2} - y_{n-3},$$
$$y_{n+2}^{(p)} = 10y_n - 20y_{n-1} + 15y_{n-2} - 4y_{n-3},$$
$$y_{n+3}^{(p)} = 20y_n - 45y_{n-1} + 36y_{n-2} - 10y_{n-3}.$$

The $A(\alpha)-$ESDIBBDF method runs by the *PECE* mode, where P indicate an application of the predictor, C is the corrector, and E is an evaluation of f. Following [14],

Definition 2. *The linear difference operator (4) is said to be of order p if*

$$C_0 = C_1 = \ldots = C_p = 0, \qquad C_{p+1} \neq 0.$$

Non-zero coefficients, C_{p+1}, is called the error constant.

The $A(\alpha)-$ESDIBBDF method has been proven to be of order 3, as its error constant is $C_4 \neq 0$.

III. Convergence Analysis

Convergence refers to the capability of a method to approximate the solution of differential equations with the desired level of accuracy, as emphasized in [15]. It is an essential property that must be considered during the development of a new method since a non-convergent method is likely to give increasingly meaningless approximations as the computational cost escalates due to the use of smaller step sizes. The following theorem stated the necessary conditions for convergence.

Theorem 2. *An LMM is convergent if and only if it is zero stable and consistent.*

The subsequent statement shown is a standard definition of convergence that is widely known among numerical researchers in the literature.

Definition 3. *An LMM is said to be convergent if for all IVPs satisfying the conditions of uniqueness, the following holds for every* $x \in [a,b]$, *and for each solution* y_n *of the difference equation satisfying the starting conditions* $y_\mu = \eta_\mu(h)$ *for which* $\lim_{h\to 0}\eta_\mu(h) = \eta$, $\mu = 0,1,\ldots,k-1$.

Given that convergence conditions relate to the consistency of a method, the following definition of consistency is provided.

Definition 4. *An LMM is said to be consistent if it has order* $p \geq 1$.

Since the $A(\alpha)-$ESDIBBDF method satisfies Definition 4 as it is of order 3 thus, the method is consistent.

From (8),

Definition 5. *A block method is consistent if and only if*

$$(i)\ \sum_{j=0}^{k} A_j = 0, \qquad (ii)\ \sum_{j=0}^{k} jA_j = \sum_{j=0}^{k} B_j, \tag{11}$$

where A_j, B_j *are* $r\times r$ *matrices and the linear difference operator of the method is*

$$L[y(x);h] = \sum_{j=0}^{k} A_j y(x+jh) - \sum_{j=0}^{k} hB_j y'(x+jh).$$

Applying Definition 5 with the values of A_j and B_j as given in (6), condition (11) of the method is

$$(i)\ \sum_{j=0}^{5} A_j = A_0 + A_1 + A_2 + A_3 + A_4 + A_5,$$

$$= \begin{bmatrix} -\frac{1}{30} \\ -\frac{1}{300} \\ \frac{1}{20} \end{bmatrix} + \begin{bmatrix} \frac{3}{20} \\ -\frac{11}{600} \\ -\frac{121}{600} \end{bmatrix} + \begin{bmatrix} -\frac{3}{10} \\ \frac{3}{25} \\ -\frac{163}{600} \end{bmatrix} + \begin{bmatrix} \frac{11}{60} \\ -\frac{169}{600} \\ -\frac{3}{40} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{11}{60} \\ -\frac{137}{600} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{11}{60} \end{bmatrix}$$

$$= 0$$

$$(ii)\ \sum_{j=0}^{5} jA_j = A_1 + 2A_2 + 3A_3 + 4A_4 + 5A_5,$$

$$= \begin{bmatrix} \frac{3}{20} \\ -\frac{11}{600} \\ -\frac{121}{600} \end{bmatrix} + 2\begin{bmatrix} -\frac{3}{10} \\ \frac{3}{25} \\ -\frac{163}{600} \end{bmatrix} + 3\begin{bmatrix} \frac{11}{60} \\ -\frac{169}{600} \\ -\frac{3}{40} \end{bmatrix} + 4\begin{bmatrix} 0 \\ \frac{11}{60} \\ -\frac{137}{600} \end{bmatrix} + 5\begin{bmatrix} 0 \\ 0 \\ \frac{11}{60} \end{bmatrix}$$

$$= \begin{bmatrix} \frac{1}{10} \\ \frac{11}{100} \\ \frac{3}{25} \end{bmatrix}$$

$$\sum_{j=3}^{5} B_j = B_3 + B_4 + B_5 = \begin{bmatrix} \frac{1}{10} \\ \frac{1}{100} \\ \frac{1}{100} \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{1}{10} \\ \frac{1}{100} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \frac{11}{60} \end{bmatrix} = \begin{bmatrix} \frac{1}{10} \\ \frac{11}{100} \\ \frac{3}{25} \end{bmatrix}$$

By satisfying condition (11), the $A(\alpha)-$ESDIBBDF method confirms its consistency. Consequently, it can be verified that the method meets the second condition for convergence, which is zero stability that can be defined as

Definition 6. *An LMM is said to be zero stable if no root of the first stability polynomial,* $p(\zeta)$, *has modulus greater than one, and if every root with modulus one is simple.*

The stability polynomial, also known as the characteristic polynomial in certain literature, is described as follows:

Definition 7. *The characteristic polynomial of LMM in Equation (1) assumes*

$$\pi(r, h\lambda) = \rho(r) - h\lambda\phi(r) = 0,$$

where $H = h\lambda$ *and* $\lambda = \frac{\partial f}{\partial y}$ *is complex.*

Hence, the stability polynomial of $A(\alpha)-$ESDIBBDF method is written as

$$R(H) = t^3 - \frac{18}{11}t^3H - \frac{3516}{6655}t^2 + \frac{108}{121}t^3H - \frac{15516}{6655}t^2H - \frac{3051}{6655}t - \frac{216}{1331}t^3H^3 + \frac{216}{605}t^2H^2 - \frac{648}{1331}tH - \frac{8}{605} \tag{12}$$

Upon solving $R(H) = 0$, the roots of the stability polynomial of the method are obtained as $t = -0.4, 0$ and 1.

Based on Definition 6, it can be concluded that the $A(\alpha)-$ESDIBBDF method exhibits zero stability. As the method satisfies both necessary conditions outlined in Theorem 2, it is therefore considered convergent. The subsequent section provides a detailed explanation of the method's stability.

IV. Stability Analysis

Applied problems often involve systems of equations where the solutions consist of elements with significantly different rates of change. In such cases, the numerical process is governed by the property of stability. Therefore, a method is deemed valuable when it possesses a region of absolute stability.

Definition 8. *The LMM in (1) is said to be absolutely stable in a region R for a given H if and only if for that H, all the roots, $r_s = r_s H$ of the stability polynomial of the linear $k-$step method, $\pi(r,H)=\rho(r)-H\phi(r)$, satisfy $|r_s|<1$, $ks=1,2,\ldots,k$ where $H=h\lambda$ and $\rho(r)$ and $\phi(r)$ are the first and second characteristic polynomials respectively. Otherwise, the method is said to be absolutely unstable.*

Fig. 1 illustrates the region of absolute stability for LMM as referred to [12]. The figure shows that the region of absolute stability is on the left part and half of the plane as stated in Definition 9.

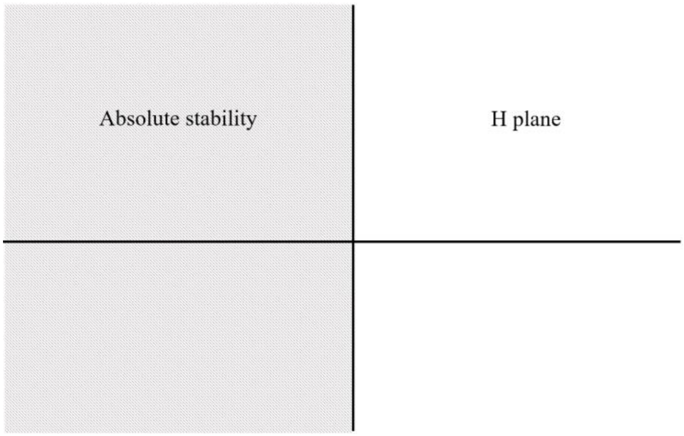

Fig. 1. The region of absolute stability for LMM.

Definition 9. *A numerical method is said to be $A-$stable if its region of absolute stability contains the whole left-hand half-plane,* $\mathrm{Re}(h\lambda)<0$.

In order to effectively solve stiff ODEs, a method must possess an $A(\alpha)-$stability, which is an essential property associated with stiffness. However, the following theorem by [14] revealed that

Theorem 3. *(i) An explicit LMM cannot be $A-$stable. (ii) The order of an $A-$stable implicit LMM cannot exceeded two. (iii) The second order $A-$stable implicit LMM with smallest error constant is the Trapezoidal rule.*

Due to the fact that the $A(\alpha)-$ESDIBBDF method is an order 3, achieving $A-$stability is not possible.

In view of this, two alternative stability properties, as defined by [17], which are more practical and suitable for the solutions of many problems are presented here.

Definition 10. *A method is stiffly stable with stiffness abscissa D if the stability region includes all complex numbers z such that* $\mathrm{Re}(z)\le -D$.

Definition 11. *A numerical algorithm is said to be $A(\alpha)-$stable for some $\alpha\in\left[0,\frac{\pi}{2}\right]$ if the region of absolute stability includes the infinite wedge*

$$S_\alpha=\{H:|Arg(-H)|<\alpha, H\neq 0\}. \tag{13}$$

The stability graph of the method is generated using Maple software. Therefore, the stability region of the $A(\alpha)-$ESDIBBDF method is given as the unshaded region of Fig. 2 with $D=0.56$ and $\alpha=65°$.

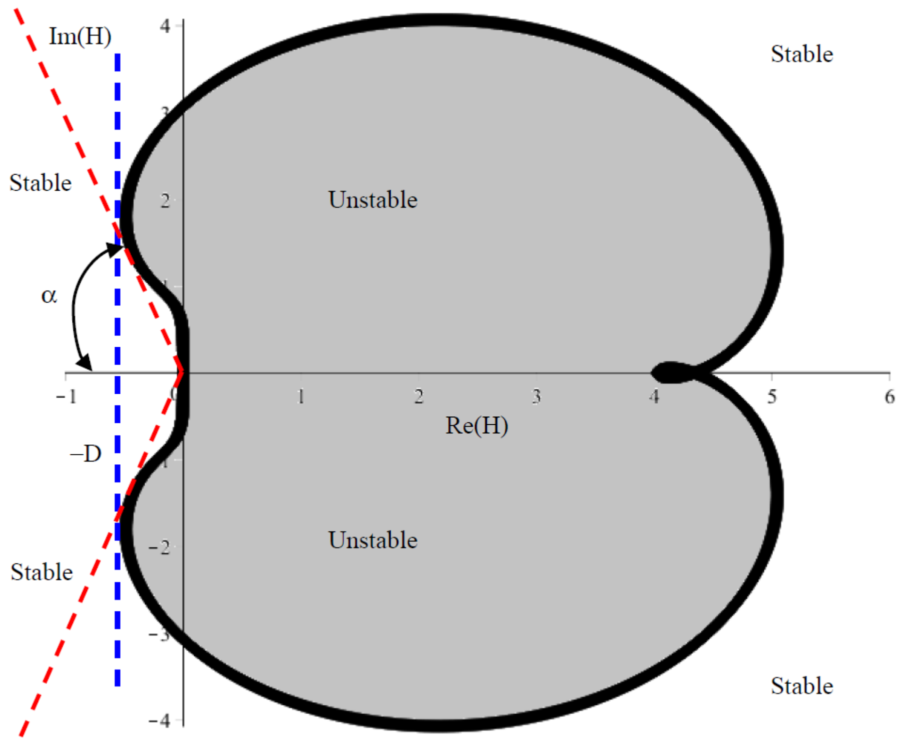

Fig. 2. The region of stiffly and $A(\alpha)-$stability of $A(\alpha)-$ESDIBBDF.

V. IMPLEMENTATION

In this section, Newton's iteration is applied to linearize formula (10) at every integration step. Let

$$F_1 = y_{n+1} - \frac{6}{11}hf_{n+1} - \zeta_1,$$
$$F_2 = y_{n+2} - \frac{6}{11}hf_{n+2} - \frac{169}{110}y_{n+1} - \frac{3}{55}hf_{n+1} - \zeta_2,$$
$$F_3 = y_{n+3} - \frac{6}{11}hf_{n+3} - \frac{137}{110}y_{n+2} - \frac{3}{55}hf_{n+2} - \frac{9}{2}y_{n+1} - \frac{3}{55}hf_{n+1} - \zeta_3.$$

with $\zeta_{1,2,3}$ are the backvalues. Then, notation i is introduced to specify the iteration as follows:

$$e_{n+1}^{(i+1)} = y_{n+1}^{(i+1)} - y_{n+1}^{(i)}, \quad e_{n+2}^{(i+1)} = y_{n+2}^{(i+1)} - y_{n+2}^{(i)}, \quad e_{n+3}^{(i+1)} = y_{n+3}^{(i+1)} - y_{n+3}^{(i)}$$

where $y^{(i+1)}$ denotes the $(i+1)^{th}$ iterative values of $y_{n+1,n+2,n+3}$, and $e_{n+1,n+2,n+3}^{(i+1)}$ denotes the differences between the $(i)^{th}$ and $(i+1)^{th}$ iterative values of $y_{n+1,n+2,n+3}$.

Thus, the Newton iteration takes the form:

$$y_{n+1}^{(i+1)} = y_{n+1}^{(i)} - \frac{F_1(y_{n+1}^{(i)})}{F_1'(y_{n+1}^{(i)})},$$
$$y_{n+2}^{(i+1)} = y_{n+2}^{(i)} - \frac{F_2(y_{n+2}^{(i)})}{F_2'(y_{n+2}^{(i)})},$$
$$y_{n+3}^{(i+1)} = y_{n+3}^{(i)} - \frac{F_3(y_{n+3}^{(i)})}{F_3'(y_{n+3}^{(i)})}.$$

The following matrix shows the computational arrangements conducted to obtain the approximations:

$$\begin{bmatrix} 1-\frac{6}{11}h\frac{\partial f_{n+1}}{\partial y_{n+1}} & 0 & 0 \\ -\frac{169}{110}-\frac{3}{55}h\frac{\partial f_{n+1}}{\partial y_{n+1}} & 1-\frac{6}{11}h\frac{\partial f_{n+2}}{\partial y_{n+2}} & 0 \\ -\frac{9}{2}-\frac{3}{55}h\frac{\partial f_{n+1}}{\partial y_{n+1}} & -\frac{137}{110}-\frac{3}{55}h\frac{\partial f_{n+2}}{\partial y_{n+2}} & 1-\frac{6}{11}h\frac{\partial f_{n+3}}{\partial y_{n+3}} \end{bmatrix} \begin{bmatrix} e_{n+1}^{(i+1)} \\ e_{n+2}^{(i+1)} \\ e_{n+3}^{(i+1)} \end{bmatrix}$$

$$= \begin{bmatrix} -1 & 0 & 0 \\ \frac{169}{110} & -1 & 0 \\ \frac{9}{2} & \frac{137}{110} & -1 \end{bmatrix} \begin{bmatrix} y_{n+1}^{(i)} \\ y_{n+2}^{(i)} \\ y_{n+3}^{(i)} \end{bmatrix} + h \begin{bmatrix} \frac{6}{11} & 0 & 0 \\ \frac{3}{55} & \frac{6}{11} & 0 \\ \frac{3}{55} & \frac{3}{55} & \frac{6}{11} \end{bmatrix} \begin{bmatrix} f_{n+1}^{(i)} \\ f_{n+2}^{(i)} \\ f_{n+3}^{(i)} \end{bmatrix} + \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \end{bmatrix}$$

VI. NUMERICAL SIMULATION

This section focuses on performing numerical experiments involving linear and system of nonlinear stiff problems to assess the efficiency of the $A(\alpha)-$ESDIBBDF method in terms of maximum error and computational time.

Definition 12. *Let $(y_i)_t$ be the t^{th} component of estimated solution and $(y(x_i))_t$ is the t^{th} component of the exact solution at x_i of (10) respectively. Then, the absolute error is given by*

$$((\text{error})_i)_t = |(y_i)_t - (y(x_i))_t|.$$

Maximum error of the method is computed as

$$MAXE = \max_{1\le i\le T}(\max_{1\le i\le N}(\text{error})_i)_t,$$

where T is the total number of steps whereas N is the number of equations.

Table 1 to 4 represent the numerical results obtained from the derived method in comparison to existing solvers. The subsequent notations have been employed:

$A(\alpha)-$ESDIBBDF	:	$A(\alpha)-$Extended Singly Diagonally Implicit BBDF
BBDF(3) $-\alpha$	:	Block Backward Differentiation $\alpha-$Formulas of order 3 by [18]
FI3BBDF	:	Fully Implicit 3-Point Block Backward Differentiation Formulas by [8]
ode15s	:	Variable step variable order solver based on the numerical differentiation formulas by MATLAB
ode23s	:	Modified Rosenbrock formula of order 2 by MATLAB
h	:	Step size
MAXE	:	Maximum error
AVE	:	Average error
TIME	:	Computational time

Test Problem 1 (Linear equation):

$$y' = -10y + 10$$

with initial condition of $y(0) = 2$ for the interval of $0 \le x \le 10$.

Exact solution: $y(x) = 1 + e^{-10x}$

Eigenvalue: $\lambda = -10$

Source: Artificial problem.

Test Problem 2 (System of linear equation):

$$y_1' = 9y_1 + 24y_2 + 5\cos x - \frac{1}{3}\sin x,,$$
$$y_2' = -24y_1 - 51y_2 - 9\cos x + \frac{1}{3}\sin x,$$

with initial conditions of $y(0) = \left(\frac{4}{3}, \frac{2}{3}\right)$ over $x \in [0,10]$.

Exact solution: $y_1(x) = 2e^{-3x} - e^{-39x} + \frac{1}{3}\cos x,$

$y_2(x) = -e^{-3x} + 2e^{-39x} - \frac{1}{3}\cos x$

Eigenvalues: $\lambda_1 = -3,\ \lambda_2 = -39$

Source: [19].

Test Problem 3 (System of nonlinear equation):

$$y_1' = -1002y_1 + 1000y_2^2,$$
$$y_2' = y_1 - y_2(1+y_2),$$

with initial conditions of $y(0) = (1,1)$ over $x \in [0,20]$.

Exact solution: $y_1(x) = e^{-2x}$, $y_2(x) = e^{-x}$

Eigenvalues: $\lambda_1 = -1,\ \lambda_2 = -2$

Source: [20].

Test Problem 4 (Chemistry problem by Robertson):

$$y_1' = -0.04y_1 + 10^4 y_2 y_3,$$
$$y_2' = 0.04y_1 - 10^4 y_2 y_3 - 3\times10^7\, y_2^2,$$
$$y_3' = 3\times10^7\, y_2^2,$$

with initial conditions $y(0) = (1,0,0)$ at the interval of $0 \le x \le 10$.

Eigenvalue: $\lambda \approx -2000$

Source: [21].

Table 1 and 2 represent numerical results when the $A(\alpha)-$ESDIBBDF method is solving linear stiff ODEs problems with different step sizes. The results are compared with compatible existing methods in terms of accuracy (MAXE) and computational time (TIME). The numerical results presented are illustrated as accuracy curves in Figure 3 and 5, and as efficiency curves in Figure 4 and 6.

TABLE 1
NUMERICAL RESULTS FOR TEST PROBLEM 1

h	METHOD	MAXE	TIME
10^{-2}	**$A(\alpha)-$ESDIBBDF**	**1.57520e-02**	**5.74144e-06**
	BBDF(3) $-\alpha$	2.66015e-02	3.01573e-05
	FI3BBDF	7.46115e-02	6.20203e-05
10^{-4}	**$A(\alpha)-$ESDIBBDF**	**1.77907e-06**	**5.06323e-05**
	BBDF(3) $-\alpha$	1.47613e-05	2.54289e-04
	FI3BBDF	1.10060e-03	5.93956e-04
10^{-6}	**$A(\alpha)-$ESDIBBDF**	**1.78097e-10**	**3.97866e-03**
	BBDF(3) $-\alpha$	1.64619e-09	2.18970e-02
	FI3BBDF	1.10361e-05	5.90466e-02

TABLE 2
NUMERICAL RESULTS FOR TEST PROBLEM 2

h	METHOD	MAXE	TIME
10^{-2}	**$A(\alpha)-$ESDIBBDF**	**2.88653e-01**	**4.71617e-05**
	BBDF(3) $-\alpha$	1.57000e-01	5.93021e-04
	FI3BBDF	1.22995e-01	8.90275e-04
10^{-4}	**$A(\alpha)-$ESDIBBDF**	**5.37948e-05**	**6.12751e-04**
	BBDF(3) $-\alpha$	1.40000e-03	1.83490e-03
	FI3BBDF	8.45420e-03	4.88259e-03
10^{-6}	**$A(\alpha)-$ESDIBBDF**	**5.40211e-09**	**7.25020e-02**
	BBDF(3) $-\alpha$	1.45000e-07	1.83291e-01
	FI3BBDF	8.54545e-05	4.68624e-01

TABLE 3
NUMERICAL RESULTS FOR TEST PROBLEM 3

h	METHOD	MAXE	AVE
10^{-2}	**$A(\alpha)-$ESDIBBDF**	**1.99039e-02**	**2.00350e-02**
	ode15s	5.20000e-03	8.71630e-04
	ode23s	1.10000e-03	3.36260e-04
10^{-4}	**$A(\alpha)-$ESDIBBDF**	**7.42129e-08**	**1.29827e-07**
	ode15s	8.55060e-05	1.51720e-05
	ode23s	2.82340e-05	1.37830e-05
10^{-6}	**$A(\alpha)-$ESDIBBDF**	**2.60030e-11**	**1.82370e-11**
	ode15s	1.07900e-06	1.27240e-07
	ode23s	5.76920e-07	6.71150e-07

TABLE 4
NUMERICAL RESULTS FOR TEST PROBLEM 4

h	METHOD	y_1	y_2	y_3
10^{-2}	**$A(\alpha)-$ESDIBBDF**	**3.39132e+02**	**4.73979e+00**	**2.86203e+01**
	ode15s	1.74768e-02	1.75038e-07	4.45546e-03
	ode23s	1.74566e-02	1.74705e-07	4.46974e-03
10^{-4}	**$A(\alpha)-$ESDIBBDF**	**1.46530e-06**	**5.34398e-09**	**6.33550e-07**
	ode15s	1.74840e-02	1.75169e-07	4.45557e-03
	ode23s	1.74723e-02	1.75240e-07	4.45215e-03
10^{-6}	**$A(\alpha)-$ESDIBBDF**	**7.04146e-07**	**1.99246e-11**	**1.27377e-07**
	ode15s	1.74950e-02	1.75599e-07	4.44233e-03
	ode23s	1.74877e-02	1.75097e-07	4.44364e-03

Based on the results, the proposed method has better accuracy than the comparing methods. Accuracy of the solutions is getting better when smaller step sizes are used as analysed in Figure 3 and 5. This is due to the higher number of function evaluations which contributes to better accuracy. By observing the efficiency curves in Figure 4 and 6, the $A(\alpha)-$ESDIBBDF method is able to compute solutions more efficiently compared to the existing methods. This is explained by the nature of the method which is in the singly diagonally implicit form instead of fully implicit.

Meanwhile, for the numerical results in Table 3 and 4, the methods are tested with a system of nonlinear problem and the well-known Chemistry problem by Robertson which has a highly stiff behaviour that models the kinetics of a chemical reaction. By referring to [22], the problem has only a single stiff eigenvalue which is almost to -2000. These problems are the ideal indicators to measure the performance of a method as a stiff solver. Therefore, for these experiments, the proposed method is compared with ode15s and ode23s, the MATLAB solvers for stiff problems. Since the program for $A(\alpha)-$ESDIBBDF method is running using a C++ software, thus the TIME between the two Mathematical software will not be considered as it is not a fair comparison.

By referring to Table 3 and 4, it can be analysed that the ode15s and ode23s have comparable accuracy. These results can be clearly observed in the accuracy curves of the numerical results presented in Figure 7 and 9. When solving for the highly stiff problem as shown in Table 4, both solvers are able to compute the solutions better than the proposed method when a bigger step size of $h = -0.01$ is used.

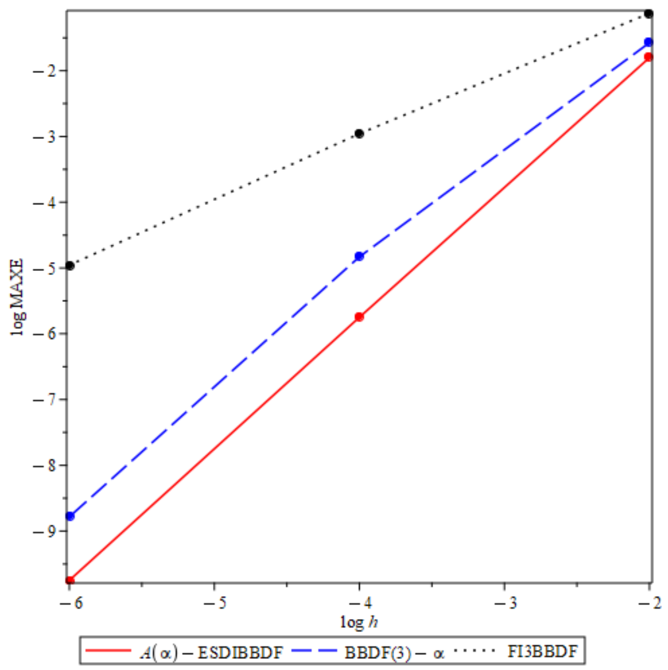

Fig. 3. Accuracy curves for Test Problem 1

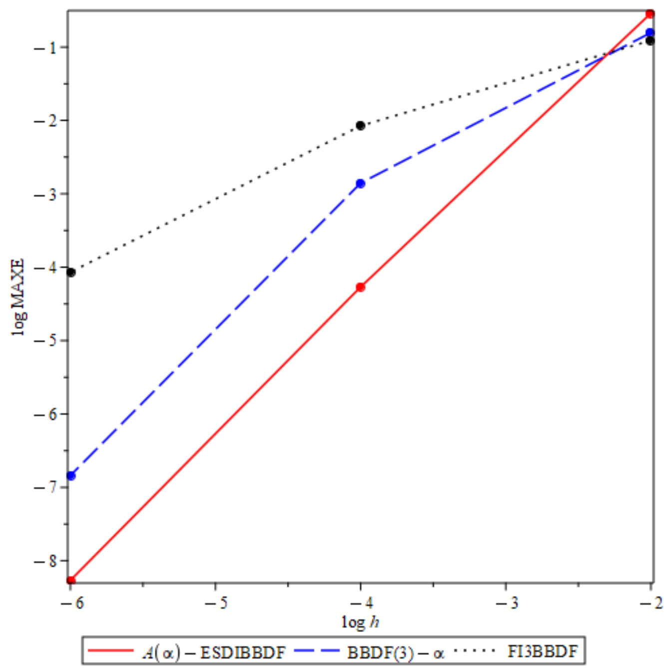

Fig. 5. Accuracy curves for Test Problem 2

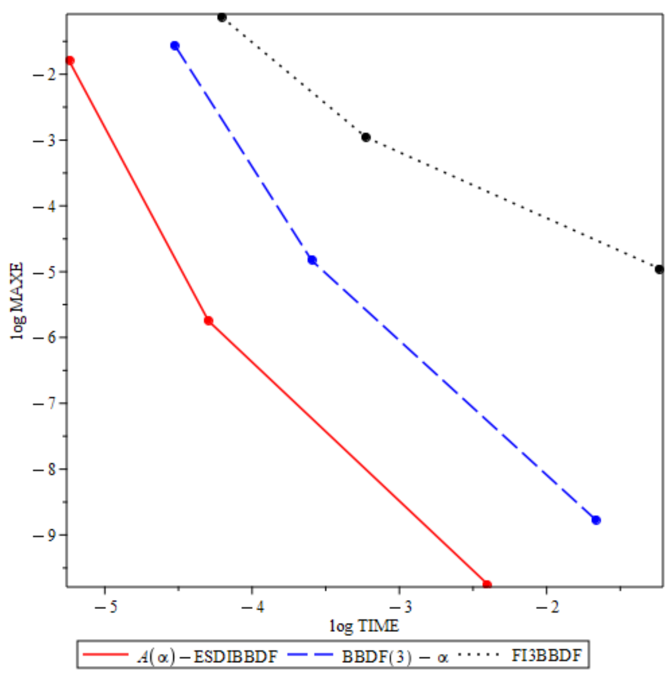

Fig. 4. Efficiency curves for Test Problem 1

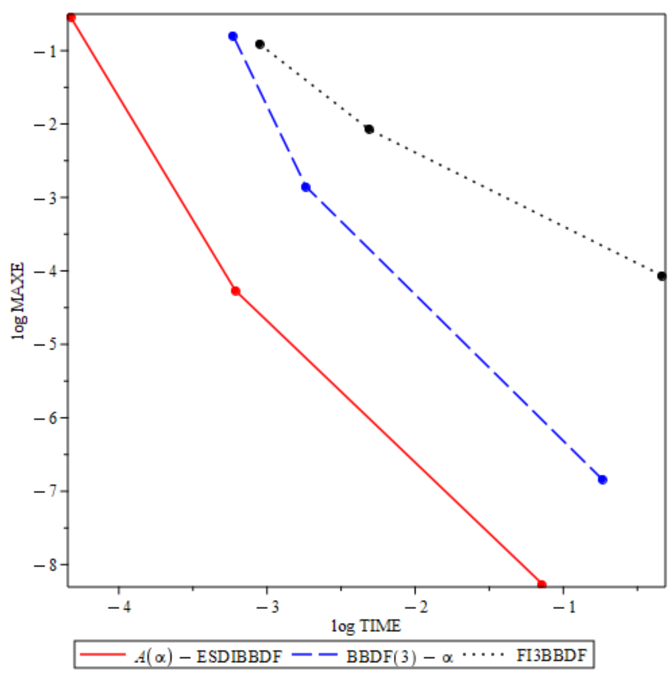

Fig. 6. Efficiency curves for Test Problem 2

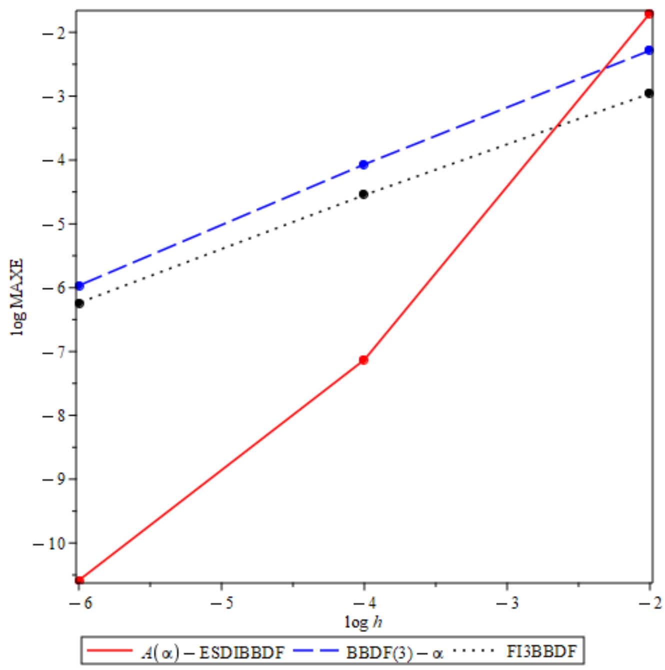

Fig. 7. Accuracy curves for Test Problem 3

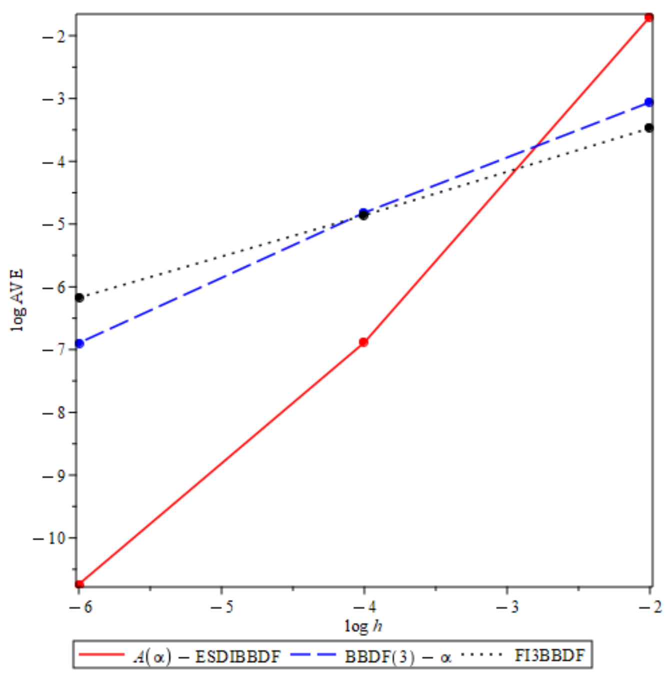

Fig. 8. Efficiency curves for Test Problem 3

However, in Figure 9, better accuracy is shown by the proposed method for each iteration point as the step sizes are getting smaller while there is no significant improvement shown by both solvers.

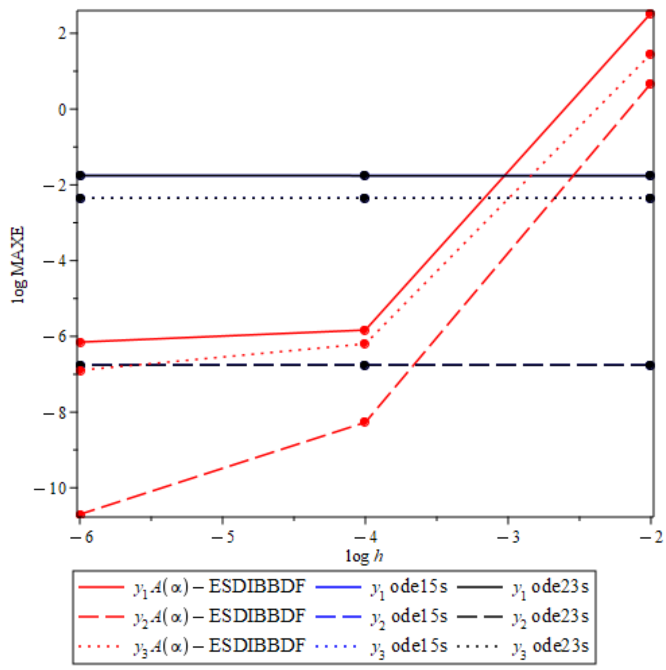

Fig. 9. Accuracy curves for Test Problem 4

VII. Conclusion

In this paper, the three points $A(\alpha)-$ESDIBBDF method of order three for solving the first order stiff ODEs is successfully developed. The method implements the strategy Error norm minimization technique for better accuracy is also considered when the method is developed.

The two necessary conditions for the convergence of the method, consistency and zero stability, are analysed in this study. The stability graph of the method verified that the method does not fulfil the $A(\alpha)-$stable property. Though, it is satisfying the stiffly stable and $A(\alpha)-$stable properties to ensure that the method is capable to solve for stiff problems.

The numerical results obtained justified the capability of the derived method to efficiently solve linear, nonlinear, and highly stiff ODEs as it produced better accuracy within a shorter time compared to the existing methods, and are able to compete well with the Mathematical software.

In conclusion, the $A(\alpha)-$ESDIBBDF method presents itself as a viable alternative solver for stiff ODEs.

To extend the research, one could apply the method for solving applied problems with stiff behaviour, to develop the method in higher order nature or with variable a step size.

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