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Stiffly Stable Diagonally Implicit Block Backward Differentiation Formula with Adaptive Step Size Strategy for Stiff Ordinary Differential Equations

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Abstract Experimental and theoretical evidence has shown that adaptive step size methods such as the backward differentiation formula (BDF) are more robust over a wider range of step sizes compared to those used in fixed step methods. Acknowledging the computational efficiency and accuracy obtained with such strategies, an adaptive step size version of the block backward differentiation formula (BBDF) in a diagonally implicit structure is proposed for solving stiff ordinary differential equations (ODEs), particularly in addressing the challenges posed by the chemical reaction problem within the domains of applied and industrial mathematics. The diagonally implicit structure with a lower triangular matrix and constant diagonal inputs offers significant advantages in evaluating the Jacobian and the lower-upper decomposition. The stability properties that were investigated show that the new class is zero$-$stable, A_0-stable and almost $A-$stable. Comparative evaluations reveal the superior performance of the proposed method compared to the existing fully implicit BBDF and ode15s conducted in MATLAB software.

Keywords adaptive step size; $\rho-$type; block backward differentiation formula; diagonally implicit; stiff stability.

Mathematics Subject Classification 34A12, 65L04, 65L05, 65L06, 65L20.

1 Introduction

Stiff ordinary differential equations (ODEs) are vital in simulating physical systems for science and engineering applications, including control theory, insulator physics, nuclear reactor theory, electrical circuits, chemical pyrolysis, chemical kinetics, molecular dynamics, reactor kinetics and chemical reactions. These problems arise when different ODE components have varying spatial dependencies. Additionally, chemical reaction problems are a crucial aspect in this context, with stiff ODEs playing a key role in modeling and optimizing reactions, especially in chemical kinetics applications.

Consider an $s \times s$ linear system

$$\widetilde{y}' = P\widetilde{y} + \widetilde{\Psi}(t), \quad \widetilde{y}(t_0) = \widetilde{Q}, \quad t \in [t_0, t_e] \tag{1}$$

where $\widetilde{y}, \widetilde{\Psi} \in \Re^s$, $\widetilde{y}^T = (y_1, y_2, \ldots, y_s)$ and $\widetilde{Q}^T = (Q_1, Q_2, \ldots, Q_s)$. P is a constant matrix with eigenvalues, λ_a and corresponding eigenvectors, c_a for $a = 1, 2, \ldots, s$. The system in (1) becomes stiff if $Re(\lambda_a) < 0$ and $\max\limits_a |Re(\lambda_a)| \gg \min\limits_a |Re(\lambda_a)|$ where the ratio,

$$S = \frac{\max\limits_i |Re(\lambda_i)|}{\min\limits_i |Re(\lambda_i)|}$$

is called the stiffness ratio or stiffness index, as defined in [1].

There exists a considerable body of literature on improving the accuracy and stability characteristics of the conventional BDF while maintaining its structure. Cash in [2] derived the extended BDF by introducing a future point to increase the order of accuracy. Later in 1981, [3] presented a class of $(p+2)-$step BDF of order p. The two extra degrees of freedom leaves some free parameters to the formula that leads to improving the absolute stability properties. The $\alpha-$type of variable step variable formula (VSVF) has been developed by Zlatev and Thomsen in [4]. Since the $\alpha-$type VSVF which is a generalization of the Adams formula that gives an excellent stability property and improved accuracy on solving non-stiff ODEs, [5] extended the implementation of $\alpha-$type VSVF for the solution of stiff systems.

Another well-known method used for solving stiff differential equations is the fully implicit of Runge-Kutta (FIRK) methods, which evaluate the Jacobian matrix,

$$J = \frac{\partial F}{\partial Y}\left(Y_{j+k}^{(i)}\right)$$

and perform the lower-upper (LU) factorization of the matrix $I - ha_{ii}\frac{\partial F}{\partial y}$ in each of its integration stage. Therefore, the authors in [6–8] chose to incorporate the lower triangular matrix with a constant value on the diagonal due to the high expense associated with implementing the FIRK methods. The aforementioned methodologies are commonly referred to as diagonally implicit Runge-Kutta (DIRKs) techniques, wherein the evaluation of J can be performed just once per step. According to Butcher in [9], it has been suggested that if the Jacobian varies sufficiently, it can be almost as effective as evaluating the Jacobian once for every stage.

This findings align with previous literature indicating that adaptive step size methods such as BDF, discussed in [10] and the second derivative linear multistep methods of [11] exhibit better performance in a wider range of step sizes than the fixed step methods (see [12]). According to [9], on deciding which step size to be used in each new step, it is necessary to employ a wise strategy in determining whether to accept or reject the previous step. Another critical condition is the inclusion of a safety factor (less than 1) in the computation to mitigate the risk of rejection in a new step. In addition, the step size ratio is typically forced to lie between two boundaries, such as 0.5 and 2.0, for the purpose to prevent a significant variation of the step size. In order to monitor the step size and optimize the method efficiency, the step ratio in a block, $r = 1, 2, \frac{5}{8}$, were considered by [13,15,16]. Encouraged by the reliability of the approach to choosing the r values, we would use $r = 1$ to retain the step size, $r = 2$ to reduce the step size to $\frac{1}{2}$ and $r = \frac{5}{8}$ to increase the step size by $\frac{8}{5}$.

It was priorly shown that BBDF is applied to solving stiff ODEs at high accuracy (see [7,13,14,17–19]). However, the theoretical stability analysis has been less focused. In realizing the full potential of the newly established method, we provide the proving of the stability properties theoretically. In a previous study [20], an analysis was conducted on the stability properties of the fixed step formula. The findings remain valid upon the selection of the free parameter, $\rho = -\frac{3}{4}$ into such method. Since this selection offers advantages compared to other existing BBDF methods, we extend the framework in adaptive step size accordingly and develop a new class of $\rho-$type formula that improves the work of [20] and [21].

The rest of the paper is structured accordingly. In Section 2, we presented the formulation of the proposed method. The stability analysis and the relevant proof are discussed in Section 3. The implementation of the method is outlined in Section 4. Numerical experiments are presented in Section 5. The conclusion is finally presented in Section 6.

2 Derivation of 2−point $\rho-$type Adaptive Step Diagonally Implicit BBDF

Let y_j denote an approximation to the theoretical solution $y(t_j)$ of (1) at t_j and $f_j = f(t_j, y_j)$. As previously stated in [1], when a numerical method is employed to determine the sequence of y_j, it takes the form of a linear relationship between y_{j+k}, f_{j+k}, where $k = 0, 1, \ldots, m$. This relationship is defined as $m-$step linear multistep method (LMM) of the following form:

$$\sum_{k=0}^{p} \upsilon_k y_{j+k} = h \sum_{k=0}^{p} \omega_k f_{j+k}. \tag{2}$$

In (2), if $\omega_0 = \omega_1 = \ldots = \omega_{p-1} = 0$ and $\omega_p \neq 0$, the resulting multistep formula is the BDF of order p and denoted as BDF$-p$.

Consider the $m-$step 2−point block LMM of fully implicit BBDF in [21]

$$\sum_{k=0}^{m} \upsilon_{k-2,p} y_{j+k-2} = h\omega_{p,p} f_{j+p}, \quad p = 1, 2 \tag{3}$$

where h is the adaptive step size used and $p = 1, 2$ are notation for y_{j+1} and y_{j+2}, respectively. The 2−point $\rho-$type adaptive step diagonally implicit block backward differentiation formula ($\rho-$ASDIBBDF) is an $m-$step LMM with $\omega_{p-1,p}$, $\omega_{p,p} \neq 0$ and $\omega_{p-1,p} = -\rho\omega_{p,p}$ for $-1 < \rho < 1$ given by

$$\sum_{k=0}^{p+m-1} \upsilon_{k-2,p} y_{j+k-2} = h\omega_{p,p} \left[f_{j+p} - \rho f_{j+p-1} \right], \quad p = 1, 2 \tag{4}$$

where $m = 3$. By taking arbitrary $\omega_{p-1,p} \neq 0$ and inserting a parameter ρ, we acquire a class of $\rho-$ASDIBBDF which incorporates the BBDF as a subset.

It should be noted that $f_{j+p} = y'(t_j + ph)$ is evaluated by using the Lagrange interpolating polynomial, $P(t)$ where $y(t) \equiv P(t)$. In order to formulate the approximation values of y_{j+1}

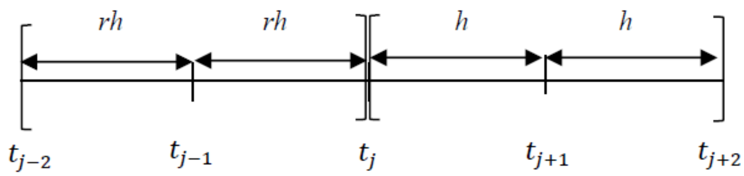


Figure 1: Interpolating points of $\rho-$ASDIBBDF

and y_{j+2}, we consider $2h$ as the step size of the computed block and $2rh$ as the step size of the previous block, where r is the step size ratio as presented in Figure 1.

The associated Lagrange polynomial for y_{j+1} which interpolates $y_{j-2}, y_{j-1}, y_j, y_{j+1}$ is given by

$$\begin{aligned} P(t) = &\frac{(t-t_{j-1})(t-t_j)(t-t_{j+1})}{(t_{j-2}-t_{j-1})(t_{j-2}-t_j)(t_{j-2}-t_{j+1})} y_{j-2} + \frac{(t-t_{j-2})(t-t_j)(t-t_{j+1})}{(t_{j-1}-t_{j-2})(t_{j-1}-t_j)(t_{j-1}-t_{j+1})} y_{j-1} \\ &+ \frac{(t-t_{j-2})(t-t_{j-1})(t-t_{j+1})}{(t_j-t_{j-2})(t_j-t_{j-1})(t_j-t_{j+1})} y_j + \frac{(t-t_{j-2})(t-t_{j-1})(t-t_j)}{(t_{j+1}-t_{j-2})(t_{j+1}-t_{j-1})(t_{j+1}-t_j)} y_{j+1}. \end{aligned} \tag{5}$$

By substituting $t = t_{j+1} + sh$, yields

$$\begin{aligned} P(t) = &\frac{s(1+s)(1+r+s)}{2r^2(-1-2r)} y_{j-2} - \frac{s(1+s)(1+2r+s)}{r^2(-1-r)} y_{j-1} - \frac{s(1+r+s)(1+2r+s)}{2r^2} y_j \\ &+ \frac{(1+s)(1+r+s)(1+2r+s)}{(1+r)(1+2r)} y_{j+1}. \end{aligned} \tag{6}$$

Differentiating (6) with respect to the variable s, gives

$$\begin{aligned} P'(t) = &-\frac{2r^2s + 3rs^2 + r^2 + 6rs + 3s^2 + 2r + 4s + 1}{2r^2(1+r)(1+2r)} y_{j-2} \\ &+ \frac{16r^2s + 12rs^2 + 8r^2 + 24rs + 6s^2 + 8r + 8s + 2}{2r^2(1+r)(1+2r)} y_{j-1} \\ &- \frac{4r^4 + 12r^3s + 6r^2s^2 + 12r^3 + 26r^2s + 9rs^2 + 13r^2 + 18rs + 3s^2 + 6r + 4s + 1}{2r^2(1+r)(1+2r)} y_j \\ &+ \frac{4r^4 + 12r^3s + 6r^2s^2 + 12r^3 + 12r^2s + 6r^2}{2r^2(1+r)(1+2r)} y_{j+1}. \end{aligned} \tag{7}$$

To obtain hf_{j+1} and hf_j in (4), we set $s = 0$ and $s = -1$, respectively in (7). This gives

$$P'(t) = hf_{j+1} = -\frac{1+r}{2r^2(1+2r)} y_{j-2} + \frac{1+2r}{r^2(1+r)} y_{j-1} - \frac{2r^2+3r+1}{2r^2} y_j + \frac{2r^2+6r+3}{(1+r)(1+2r)} y_{j+1} \tag{8}$$

$$P'(t) = hf_j = \frac{1}{2r(1+2r)} y_{j-2} - \frac{2}{r(1+r)} y_{j-1} - \frac{3-2r}{2r} y_j + \frac{2r^2}{(1+r)(1+2r)} y_{j+1} \tag{9}$$

and upon solving $(hf_{j+1} - \rho hf_j)$ from (8) and (9) for y_{j+1}, we obtain

$$\begin{aligned} y_{j+1} = &-\frac{r^2\rho + r^2 + r\rho + 2r + 1}{2r^2(2r^2\rho - 2r^2 - 6r - 3)} y_{j-2} + \frac{8r^2\rho + 8r^2 + 4r\rho + 8r + 2}{2r^2(2r^2\rho - 2r^2 - 6r - 3)} y_{j-1} \\ &+ \frac{4r^4\rho - 4r^4 - 12r^3 - 7r^2\rho - 13r^2 - 3r\rho - 6r - 1}{2r^2(2r^2\rho - 2r^2 - 6r - 3)} y_j \\ &+ \frac{4r^4 + 6r^3 + 2r^2}{2r^2(2r^2\rho - 2r^2 - 6r - 3)} \rho hf_j - \frac{4r^4 + 6r^3 + 2r^2}{2r^2(2r^2\rho - 2r^2 - 6r - 3)} hf_{j+1}. \end{aligned} \tag{10}$$

The approximation for y_{j+2} is obtained by generating $P(t)$ that interpolates $y(t)$ at points $t_{j-2}, t_{j-1}, t_{j+1}, t_{j+2}$; that is

$$\begin{aligned} P(t) = &\frac{(t - t_{j-1})(t - t_{j+1})(t - t_{j+2})}{(t_{j-2} - t_{j-1})(t_{j-2} - t_{j+1})(t_{j-2} - t_{j+2})} y_{j-2} + \frac{(t - t_{j-2})(t - t_{j+1})(t - t_{j+2})}{(t_{j-1} - t_{j-2})(t_{j-1} - t_{j+1})(t_{j-1} - t_{j+2})} y_{j-1} \\ &+ \frac{(t - t_{j-2})(t - t_{j-1})(t - t_{j+2})}{(t_{j+1} - t_{j-2})(t_{j+1} - t_{j-1})(t_{j+1} - t_{j+2})} y_{j+1} + \frac{(t - t_{j-2})(t - t_{j-1})(t - t_{j+1})}{(t_{j+2} - t_{j-2})(t_{j+2} - t_{j-1})(t_{j+2} - t_{j+1})} y_{j+2}. \end{aligned} \tag{11}$$

In a similar manner, by defining $t = t_{j+2} + sh$ and on solving $(hf_{j+2} - \rho hf_{j+1})$ for y_{j+2}, gives

$$\begin{aligned} y_{j+2} = &-\frac{r^2\rho + r^2 + 3r\rho + 4r + 2\rho + 1}{r(1 + 2r)(2r^2\rho - 2r^2 + 3r\rho - 9r + \rho - 8)} y_{j-2} \\ &+ \frac{8r^2\rho + 8r^2 + 8r\rho + 12r + 2\rho + 4}{r(1 + 2r)(2r^2\rho - 2r^2 + 3r\rho - 9r + \rho - 8)} y_{j-1} \\ &+ \frac{4r^4\rho - 4r^4 - 8r^3\rho - 20r^3 - 2r^2\rho - 32r^2 - 4r\rho - 16r}{r(1 + 2r)(2r^2\rho - 2r^2 + 3r\rho - 9r + \rho - 8)} y_{j+1} \\ &- \frac{4r^4 + 14r^3 + 14r^2 + 4r}{r(1 + 2r)(2r^2\rho - 2r^2 + 3r\rho - 9r + \rho - 8)} hf_{j+2} \\ &+ \frac{4r^4 + 14r^3 + 14r^2 + 4r}{r(1 + 2r)(2r^2\rho - 2r^2 + 3r\rho - 9r + \rho - 8)} \rho hf_{j+1}. \end{aligned} \tag{12}$$

Next, the coefficients of $\upsilon_{k-2,p}$ and $\omega_{p,p}$ in (10) and (12) are substituted into (4) to obtain the corresponding corrector formula of 2−point $\rho-$ASDIBBDF for $r = 1, 2, \frac{5}{8}$ as presented in Table 1. The predictor formula for y_{j+1} and y_{j+2} are computed using t_{j-2}, t_{j-1} and t_j as the interpolating points, and are provided as follows (see [21]),

(a) for $r = 1$,
$y_{j+1} = y_{j-2} - 3y_{j-1} + 3y_j, \quad y_{j+2} = 3y_{j-2} - 8y_{j-1} + 6y_j,$

(b) for $r = 2$,
$y_{j+1} = \frac{3}{8}y_{j-2} - \frac{5}{4}y_{j-1} + \frac{15}{8}y_j, \quad y_{j+2} = y_{j-2} - 3y_{j-1} + 3y_j,$

(c) for $r = \frac{5}{8}$,
$y_{j+1} = \frac{52}{25}y_{j-2} - \frac{144}{25}y_{j-1} + \frac{117}{25}y_j, \quad y_{j+2} = \frac{168}{25}y_{j-2} - \frac{416}{25}y_{j-1} + \frac{273}{25}y_j.$

Table 1: Formula for 2−point ρ−ASDIBBDF

r	Corrector formula
1	$y_{j+1} = -\dfrac{\rho+2}{2\rho-11}y_{j-2} + \dfrac{6\rho+9}{2\rho-11}y_{j-1} - \dfrac{3\rho+18}{2\rho-11}y_j + \dfrac{6\rho}{2\rho-11}hf_j - \dfrac{6}{2\rho-11}hf_{j+1}$
	$y_{j+2} = -\dfrac{2\rho+3}{6\rho-19}y_{j-2} + \dfrac{6\rho+8}{6\rho-19}y_{j-1} + \dfrac{2\rho-24}{6\rho-19}y_{j+1} + \dfrac{12\rho}{6\rho-19}hf_{j+1} - \dfrac{12}{6\rho-19}hf_{j+2}$
2	$y_{j+1} = -\dfrac{1}{8}\left(\dfrac{6\rho+9}{8\rho-23}\right)y_{j-2} + \dfrac{5}{4}\left(\dfrac{4\rho+5}{8\rho-23}\right)y_{j-1} + \dfrac{5}{8}\left(\dfrac{6\rho+45}{8\rho-23}\right)y_j + \dfrac{15\rho}{8\rho-23}hf_j - \dfrac{15}{8\rho-23}hf_{j+1}$
	$y_{j+2} = -\dfrac{2}{5}\left(\dfrac{3\rho+4}{15\rho-34}\right)y_{j-2} + \dfrac{5\rho+6}{15\rho-34}y_{j-1} + \dfrac{2}{5}\left(\dfrac{28\rho-96}{15\rho-34}\right)y_{j+1} + \dfrac{24\rho}{15\rho-34}hf_{j+1} - \dfrac{24}{15\rho-34}hf_{j+2}$
$\dfrac{5}{8}$	$y_{j+1} = -\dfrac{32}{25}\left(\dfrac{\frac{65}{64}\rho+\frac{169}{64}}{\frac{25}{32}\rho-\frac{241}{32}}\right)y_{j-2} + \dfrac{64}{25}\left(\dfrac{\frac{45}{16}\rho+\frac{81}{16}}{\frac{25}{32}\rho-\frac{241}{32}}\right)y_{j-1} + \dfrac{32}{25}\left(\dfrac{-\frac{4095}{1024}\rho-\frac{13689}{1024}}{\frac{25}{32}\rho-\frac{241}{32}}\right)y_j + \dfrac{117\rho}{32\left(\frac{25}{32}\rho-\frac{241}{32}\right)}hf_j - \dfrac{117}{32\left(\frac{25}{32}\rho-\frac{241}{32}\right)}hf_{j+1}$
	$y_{j+2} = -\dfrac{32}{45}\left(\dfrac{\frac{273}{64}\rho+\frac{441}{64}}{\frac{117}{32}\rho-\frac{461}{32}}\right)y_{j-2} + \dfrac{16}{5}\left(\dfrac{\frac{9}{4}\rho+\frac{13}{4}}{\frac{117}{32}\rho-\frac{461}{32}}\right)y_{j-1} + \dfrac{8}{9}\left(\dfrac{-\frac{147}{256}\rho-\frac{5733}{256})}{\frac{117}{32}\rho-\frac{461}{32}}\right)y_{j+1} + \dfrac{273\rho}{32\left(\frac{117}{32}\rho-\frac{461}{32}\right)}hf_{j+1} - \dfrac{273}{32\left(\frac{117}{32}\rho-\frac{461}{32}\right)}hf_{j+2}$

3 Analysis of Stability Properties

This section primarily investigate the stability properties of p−ASDIBBDF for $\rho \in (-1, 1)$. The values of free parameter ρ are restricted to the above said interval to ensure the stiff stability of the derived methods (see [13, 17, 20, 22]). The method adopted in this section to demonstrate specific stability properties at $p = 1, 2$ is attributable to [22]. Some important stability requirements for a numerical method are examined, including A_0−stability, zero−stability and $A(\alpha)$−stability.

3.1 A_0−Stability

For the next theorem associated with A_0−stability, the subsequent lemmas are being used.

Lemma 1 *Assume $p(t) = p_3t^3 + p_2t^2 + p_1t + p_0$, where p_i's are real values and $p_3 \neq 0$, then $p(t)$ is a Hurwitz polynomial if and only if these two conditions both hold:*

(i) *All p_i's are either positive or negative.*

(ii) $p_1p_2 - p_0p_3 > 0$.

Proof See [20]. □

Lemma 2 *Let $f(t) = at^2+bt+c$, where a, b, c are real values, $a > 0$ and $c \geq 0$. Then, $f(t) > 0$ for all $t < 0$ if and only if either $b \leq 0$ or $0 < b < 2\sqrt{ac}$.*

Proof For $a > 0$, one can observed that the quadratic graph of $f(t)$ will concave upward and the vertex is at $t_0 = -\frac{b}{2a}$ and the $y-$intercept, $c \geq 0$. If $b < 0$, the position of the vertex will be on the right of the $t-$axis. It means that, if $b < 0$, then $f(t) > 0$ for all $t < 0$. If $b = 0$, then $f(t) > 0$ for all $t \neq 0$. If $b > 0$, then the vertex will be on the left of the origin. Now, by observing the discriminant of a quadratic i.e. $b^2 - 4ac$, consider for this two cases: (i) When $b > 0$ and $b^2 - 4ac < 0$, then $f(t) > 0$ for all $t < 0$. For case (ii) When $b > 0$ and $b^2 - 4ac \geq 0$, then there exists $t_0 < 0$ such that $f(t) \leq 0$. Thus, $f(t) > 0$ for all $t < 0$ if and only if either $b \leq 0$ or $b > 0$ and $b^2 - 4ac < 0$. Case (i) is equivalent to $0 < b < 2\sqrt{ac}$. □

Definition 1 *The method is A_0-stable if $\{\mu \in \mathbb{C}| \, Im(\mu) = 0, -\infty < \mu < 0\} \subset \tilde{A}$.*

Theorem 1 *The method satisfies A_0-stability for $\rho \in (-1, 1)$ if and only if all three conditions below hold:*

(a) $\tilde{A}_1 \equiv 1 + \upsilon_{-2,p} \geq 0$,

(b) $\tilde{A}_2 \equiv 1 - 2\upsilon_{-2,p} - \upsilon_{-1,p} \geq 0$,

(c) $\tilde{A}_3 \equiv 2 - \rho\upsilon_{-2,p} - \upsilon_{-1,p} \geq 0$, *or* $-2\sqrt{\tilde{A}_1\tilde{A}_2} < \tilde{A}_3 < 0$.

Proof Given that the transformation of the Möbius maps the $\xi-$plane to the $z-$plane as shown below

$$r(z) = \left(\frac{1-z}{2}\right)^m \varrho\left(\frac{1+z}{1-z}\right), \quad s(z) = \left(\frac{1-z}{2}\right)^m \sigma\left(\frac{1+z}{1-z}\right),$$

to form $Q(z, \mu) = r(z) - \mu s(z)$ where $\mu = h\lambda$.
Remark: In solving stiff equations, the equation $y' = \lambda y$ will be considered, where $\lambda \in \mathbb{C}$ in which $\Re(\lambda) < 0$ is used. For $p = 1, 2$, the expanded polynomials can be represented as

$$\begin{aligned} 8r(z) &= 2(1 + \upsilon_{-1,p})z^3 + 4(1 + \upsilon_{-2,p})z^2 + 2(1 - 2\upsilon_{-2,p} - \upsilon_{-1,p})z, \\ 8s(z) &= \omega_{p,p}\left[(1 + \rho)z^3 + (3 + \rho)z^2 + (3 - \rho)z + (1 - \rho)\right], \end{aligned}$$

to formulate $Q(z, \mu)$ which can be simplified into

$$8Q(z, \mu) = [q_1 - \mu\omega_{p,p}(1 + \rho)]\, z^3 + [q_2 - \mu\omega_{p,p}(3 + \rho)]\, z^2 + [q_3 - \mu\omega_{p,p}(3 - \rho)]\, z - \mu\omega_{p,p}(1 - \rho),$$

where $q_1 = 2(1+\upsilon_{-1,p})$, $\quad q_2 = 4(1+\upsilon_{-2,p})$, $\quad q_3 = 2(1-2\upsilon_{-2,p}-\upsilon_{-1,p})$. Note that $\omega_{p,p} > 0$ and $\upsilon_{-1,p} > 0$, then $q_1 > 0$, $\mu\omega_{p,p}(1 - \rho) > 0$ and $-\mu\omega_{p,p}(1 + \rho) \geq 0$ for all $\mu < 0$. Thus, by Lemma 1, $Q(z, \mu)$ is a Hurwitz polynomial if and only if the following three conditions are satisfied for $\mu < 0$:

(i) $p_1 = q_3 - \mu\omega_{p,p}(3 - \rho) > 0$,

(ii) $p_2 = q_2 - \mu\omega_{p,p}(3+\rho) > 0$,

(iii) $p_1p_2 - p_0p_3 > 0$, where $p_3 = q_1 - \mu\omega_{p,p}(1+\rho)$ and $p_0 = -\mu\omega_{p,p}(1-\rho)$.

Now, by referring to (ii), $p_2 > 0$ for all $\mu < 0$ if and only if $q_2 \geq 0$ and $q_2 \geq 0$ if and only if $\upsilon_{-2,p} \geq -1$ which is condition (a) of the theorem. From (i), $p_1 > 0$ for all $\mu < 0$ if and only if $q_3 \geq 0$ and $q_3 \geq 0$ if and only if $(2\upsilon_{-2,p} + \upsilon_{-1,p}) \leq 1$ which is condition (b) of the theorem. For condition (iii), we have $p_1p_2 - p_0p_3 = 8\left(\omega_{p,p}\mu\right)^2 - 8\tilde{A}_3\left(\omega_{p,p}\mu\right) + 8\tilde{A}_1\tilde{A}_2 = \left(\omega_{p,p}\mu\right)^2 - \tilde{A}_3\left(\omega_{p,p}\mu\right) + \tilde{A}_1\tilde{A}_2$. By comparing the coefficients of $\left(\omega_{p,p}\mu\right)^2$, $\left(\omega_{p,p}\mu\right)$ and constant term $\tilde{A}_1\tilde{A}_2$ with $f(t) = at^2 + bt + c$ in Lemma 2, we can notate $a = 1, b = -\tilde{A}_3$ and $c = \tilde{A}_1\tilde{A}_2$. By Lemma 1, $p_1p_2 - p_0p_3 > 0$ for all $\mu < 0$ with $q_2 \geq 0$ and $q_3 \geq 0$ if and only if either $-\tilde{A}_3 \leq 0$ or $0 < -\tilde{A}_3 < 2\sqrt{\tilde{A}_1\tilde{A}_2}$ which is condition (c) of the theorem. The theorem satisfied all conditions in (a), (b) and (c), therefore the method is said to be A_0-stable for $\rho \in (-1, 1)$. □

3.2 Zero and $A(\alpha)-$Stability

We are interested in determining for which $h\lambda$ the derived method is zero−stable and absolutely stable, based on the the following definitions:

Definition 2 *The method in (4) is zero−stable if its characteristic polynomial has a simple root at +1 and all the remaining roots reside strictly in the closed complex unit disc (refer [23]).*

Definition 3 *The method in (4) is said to have region of absolute stability $\Re_A$, where $\Re_A$ is a region of the complex $\hat{h}-$plane, if it is absolutely stable for all $\hat{h} \in \Re_A$. The intersection of $\Re_A$ with the $x-$axis is called the interval of absolute stability (refer [24]).*

It is important to acknowledge that the absolute stability interval is applicable for the case of the Dahlquist test equation $y' = \lambda y$ and $h\lambda = \hat{h}$. The coefficients of the corrector formula in Table 1 can be expressed using this notation:

$$\underbrace{\begin{bmatrix} 1 - \dfrac{2r^2+3r+1}{\frac{7}{2}r^2+6r+3}\hat{h} & 0 \\ -\dfrac{7r^3+26r^2+\frac{61}{2}r+13}{(2r+1)\left(\frac{7}{2}+\frac{45}{4}+\frac{35}{4}\right)} - \dfrac{3}{2}\left(\dfrac{r^2+3r+2}{\frac{7}{2}+\frac{45}{4}+\frac{35}{4}}\right)\hat{h} & 1 - \dfrac{2r^2+6r+4}{\frac{7}{2}+\frac{45}{4}+\frac{35}{4}}\hat{h} \end{bmatrix}}_{A} \begin{bmatrix} y_{j+1} \\ y_{j+2} \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} -\dfrac{r^2+\frac{5}{2}r+1}{\frac{7}{2}r^4+6r^3+3r^2}\hat{h} & \dfrac{1}{2}\left(\dfrac{7r^4+12r^3+\frac{31}{4}r^2+\frac{15}{4}r+1}{\frac{7}{2}r^4+6r^3+3r^2}\right) + \dfrac{3}{4}\left(\dfrac{2r^2+3r+1}{\frac{7}{2}r^2+6r+3}\right)\hat{h} \\ -\dfrac{r+\frac{5}{2}}{\frac{7}{2}r^3+\frac{45}{4}r^2+\frac{35}{4}r} & 0 \end{bmatrix}}_{B} \tag{13}$$

$$\begin{bmatrix} y_{j-1} \\ y_j \end{bmatrix} + \underbrace{\begin{bmatrix} 0 & \dfrac{1}{2}\left(\dfrac{\frac{1}{4}r^2+\frac{5}{4}r+1}{\frac{7}{2}r^4+6r^3+3r^2}\right) \\ 0 & \dfrac{\frac{1}{4}r^2+\frac{7}{4}r+\frac{5}{2}}{(2r+1)\left(\frac{7}{2}r^3+\frac{45}{4}r^2+\frac{35}{4}r\right)} \end{bmatrix}}_{C} \begin{bmatrix} y_{j-3} \\ y_{j-2} \end{bmatrix}$$

to form $AY_J = BY_{J-1} + CY_{J-2}$ in terms of r. Table 2 presents the stability polynomial of the scalar test equation, denoted as $\pi(\acute{t}, \hat{h})$, which is used to establish the absolute stability region of the method. This polynomial is produced by evaluating the roots of $\acute{t}$, where $|A\acute{t}^2 - B\acute{t} - C| = 0$.

Table 2: Stability polynomial for $\rho-$ASDIBBDF

r	Stability polynomial
1	$\pi(\acute{t},\hat{h}) = \acute{t}^4 - \frac{1164}{1175}\acute{t}^4\hat{h} + \frac{18}{1175}\acute{t}^2 + \frac{288}{1175}\acute{t}^4\hat{h}^2 + \frac{54}{1175}\acute{t}^2\hat{h} - \frac{2367}{2350}\acute{t}^3 - \frac{1242}{1175}\acute{t}^3\hat{h} - \frac{19}{2350}\acute{t} - \frac{162}{1175}\acute{t}^3\hat{h}^2$
2	$\pi(\acute{t},\hat{h}) = \acute{t}^4 - \frac{5499}{5249}\acute{t}^4\hat{h} + \frac{1471}{83984}\acute{t}^2 + \frac{1440}{5249}\acute{t}^4\hat{h}^2 + \frac{411}{20996}\acute{t}^2\hat{h} - \frac{5339}{5249}\acute{t}^3 - \frac{9147}{10498}\acute{t}^3\hat{h} - \frac{31}{83984}\acute{t} - \frac{810}{5249}\acute{t}^3\hat{h}^2$
$\frac{5}{8}$	$\pi(\acute{t},\hat{h}) = \acute{t}^4 - \frac{2161848}{2280605}\acute{t}^4\hat{h} - \frac{778464}{57015125}\acute{t}^2 + \frac{511056}{2280605}\acute{t}^4\hat{h}^2 + \frac{3244176}{57015125}\acute{t}^2\hat{h} - \frac{53033589}{57015125}\acute{t}^3 - \frac{83130138}{57015125}\acute{t}^3\hat{h} - \frac{3203072}{57015125}\acute{t} - \frac{287469}{2280605}\acute{t}^3\hat{h}^2$

By setting $\hat{h} = 0$ and on solving the stability polynomials for $r = 1, 2, \frac{5}{8}$ in Table 2, $\pi(\acute{t}, \hat{h})$ turns out to have roots, $\acute{t}$ as listed in Table 3. Thus, by referring to Definition 2, we infer that the method is zero−stable.

Table 3: Roots of the stability polynomial of $\rho-$ASDIBBDF

r	1	2	$\frac{5}{8}$
$\acute{t}_1$	0	0	0
$\acute{t}_2$	1	1	1
$\acute{t}_3$	$0.003617 + 0.08982i$	$0.008573 + 0.01719i$	$-0.03492 + 0.2344i$
$\acute{t}_4$	$0.003617 - 0.08982i$	$0.008573 - 0.01719i$	$-0.03492 - 0.2344i$

One further drawback of a numerical method are $A(\alpha)$ (or almost $A-$stability) and stiff stability. Both properties were defined by [10] as follows:

Definition 4 *A method is stiffly stable if in the region* $R_1 = \{Re(h\lambda) \leq D\}$ *it is absolute stable and in* $R_2 = \{D < Re(h\lambda) < \alpha, |Im(h\lambda)| < \theta\}$ *it is accurate. Gear in [10] illustrate the regions of* $R_1 \cup R_2$ *in Figure 2.*

Definition 5 *A method is* $A(\alpha)-$*stable,* $\alpha \in (0, \frac{\pi}{2})$ *if all solutions of* $y' = \lambda y$ *converge to 0 as* n *tend to infinity with a fixed* h*, so that* $|arg(-\lambda)| < \alpha, |\lambda| \neq 0$*. This definition was given by [10].*

Butcher in [25] highlighted that Definitions 4 and 5 are based on the concept of stability, which suggests that there are several rigid issues with spectra that are located in the left half-plane but not close to the imaginary axis.

The definitions of stiffly stable and $A(\alpha)-$stable provided in [25] are herein stated accordingly (refer Figure 3).

Definition 6 *The method in (4) is stiffly stable with stiffness abscissa,* D *if all complex numbers* $h\lambda$ *are included in the stability region, so that* $Re(h\lambda) \leq -D$*.*

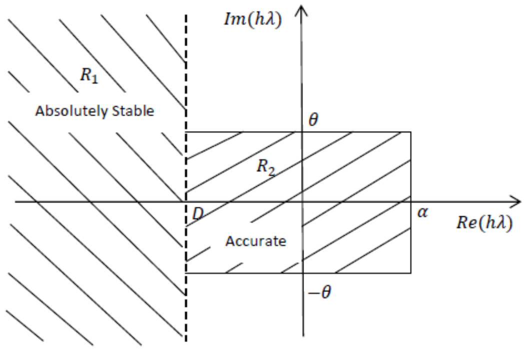


Figure 2: Stiffly stability region as illustrated in [10]

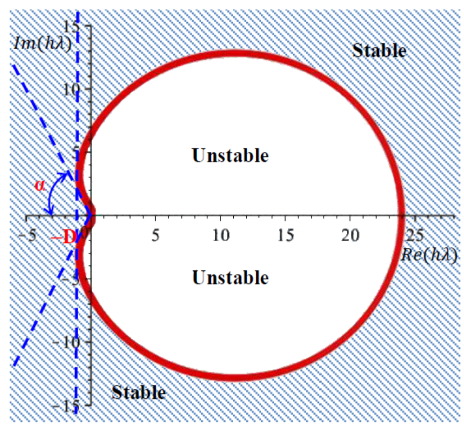


Figure 3: $A(\alpha)-$stable region as featured in [25]

Definition 7 *The method in (4) is $A(\alpha)-$stable if all complex numbers $h\lambda$ are included in the stability region, so that $-(\pi-\alpha) \leq arg(h\lambda) \leq \pi-\alpha$.*

The following theorem gives necessary and sufficient conditions for stiff stability. The related proof for y_{n+1} have been presented in [20].

Theorem 2 *The conditions* (a)–(d) are necessary and sufficient for a convergent method to be stiffly stable.

(a) The method is A_0-stable,

(b) The modulus of any root of the polynomial $\frac{\varrho(\xi)}{\xi-1}$ is less than 1,

(c) The roots of $\sigma(\xi)$ of modulus 1 are simple,

(d) If ξ_0 is a root of $\sigma(\xi)$ with $|\xi_0| = 1$, then

$$\frac{\varrho(\xi)}{\xi\sigma'(\xi)}$$

at $\xi = \xi_0$ is real and positive.

The following lemma will be used to prove Theorem 2.

Lemma 3 *Let*

$$p(x) = \tilde{a}_2 x^2 + \tilde{a}_1 x + \tilde{a}_0,$$

where $\tilde{a}_0, \tilde{a}_1, \tilde{a}_2 \neq 0$ *and* $\tilde{a}_0, \tilde{a}_1, \tilde{a}_2$ *are real. Then* $p(x)$ *is a Schur polynomial if and only if the conditions of (i) and (ii) are met.*

(i) $|\tilde{a}_0| < |\tilde{a}_2|$,

(ii) $|\tilde{a}_1| < |\tilde{a}_2 + \tilde{a}_0|$.

Proof See [22]. □

Theorem 3 *The method is strongly stable for* $\rho \in (-1, 1)$.

Proof It suffices to show that

$$\frac{\varrho(\xi)}{\xi - 1}$$

is a Schur polynomial for $\rho \in (-1, 1)$. From Table 1, $a_{-2,2} + a_{-1,2} + a_{0,2} + 1 = 0$. Polynomial $\varrho(\xi)$ can be written as $\varrho(\xi) = (\xi - 1)(\tilde{a}_2\xi^2 + \tilde{a}_1\xi + \tilde{a}_0)$. Then, by collecting the common terms of ξ in (9), we have

$$\tilde{a}_0 = -a_{-2,2} = \frac{3 + 2\rho}{19 - 6\rho}, \tilde{a}_1 = -(a_{-2,2} + a_{-1,2}) = -\left(\frac{5 + 4\rho}{19 - 6\rho}\right)$$

and $\tilde{a}_2 = 1$. Since $\frac{3+2\rho}{19-6\rho} \leq \frac{5}{13}$ for $-1 < \rho < 1$, we have $\tilde{a}_0 < \tilde{a}_2$. Now, $\tilde{a}_2 + \tilde{a}_0 = \frac{22-4\rho}{19-6\rho}$ and $|\tilde{a}_2 + \tilde{a}_0| - |\tilde{a}_1| = \frac{17-8\rho}{19-6\rho} > 0$ for $-1 < \rho < 1$. Thus, by Lemma 2, $\frac{\varrho(\xi)}{\xi-1}$ is a Schur polynomial. □

Theorem 4 *The method is stiffly stable for* $\rho \in (-1, 1)$.

Proof $\sigma(\xi) = b_{1,2}\left(\xi^3 - \rho\xi^2\right)$ where $b_{1,2} = \frac{12}{19-6\rho}$. The roots of $\sigma(\xi)$ are $0, \rho$ and it has simple root of modulus 1. Now Theorem 2 together with Theorem 1 and Theorem 3 imply that the method is stiffly stable for all $\rho \in (-1, 1)$. □

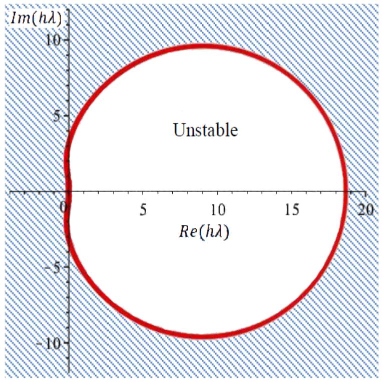
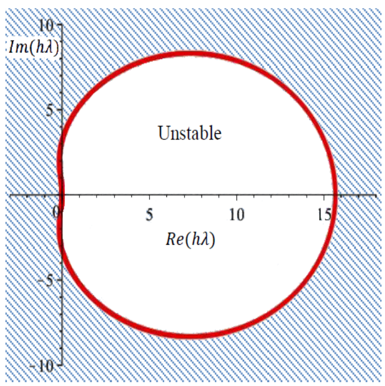
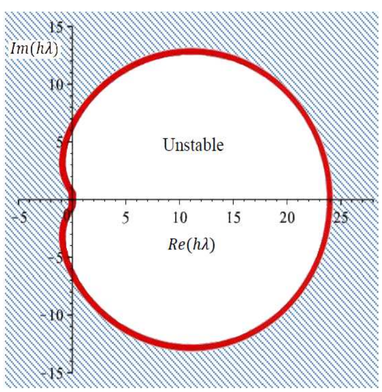
Corollary 1 *The method is* $A(\alpha)-$*stable for all* $\rho \in (-1, 1)$.

Proof Stiff stability implies $A(\alpha)-$stability (refer to [20]). □

Next, the absolute stability region is determined. The boundary of the stability region for a range of $\theta \in [0, 2\pi]$ is obtained by setting $\acute{t} = e^{i\theta}$ for which $|\acute{t}| \leq 1$ into the stability polynomial in Table 2. The absolute stability regions, intervals of unstable region, values of D and angles of α for $r = 1, 2, \frac{5}{8}$ are given in Table 4.

As depicted in Table 4, the stable region lies outside the closed contour of the graph. Thus, by Definition 7, the method for $r = 1, 2, \frac{5}{8}$ is considered $A(\alpha)-$stable.

Table 4: Absolute stability regions, $\Re_A$, intervals of unstable region, D and α of $\rho-$ASDIBBDF

r	$\Re_A$	Interval of unstable region	D	α
1		(0, 18.667)	−0.156	85.657°
2		(0, 15.825)	−0.151	85.641°
$\frac{5}{8}$		(0, 23.961)	−0.919	73.577°

4 Implementation of the Method using Newton's Iteration

An approximation of the values y_{j+1} and y_{j+2} in (4) will be generated using Newton's iteration. General formulae in Table 1 can be described as:

$$\begin{aligned} y_{j+1} &= \upsilon_{2,1}y_{j+2} + \omega_{0,1}hf_j + \omega_{1,1}hf_{j+1} + \aleph_1, \\ y_{j+2} &= \upsilon_{1,2}y_{j+1} + \omega_{1,2}hf_{j+1} + \omega_{2,2}hf_{j+2} + \aleph_2, \end{aligned} \tag{14}$$

where $\aleph_1$ and $\aleph_2$ are the back values. The matrix-vector of equation (14) is equivalent to

$$(I-\upsilon)\,Y = h\,(\Gamma_1 F_1 + \Gamma_2 F_2) + \aleph,$$

where

$$\begin{aligned} I &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \upsilon = \begin{bmatrix} 0 & \upsilon_{2,1} \\ \upsilon_{1,2} & 0 \end{bmatrix}, \Gamma_1 = \begin{bmatrix} 0 & \omega_{0,1} \\ 0 & 0 \end{bmatrix}, \Gamma_2 = \begin{bmatrix} \omega_{1,1} & 0 \\ \omega_{1,2} & \omega_{2,2} \end{bmatrix}, \\ Y &= \begin{bmatrix} y_{j+1} \\ y_{j+2} \end{bmatrix}, F_1 = \begin{bmatrix} f_{j-1} \\ f_j \end{bmatrix}, F_2 = \begin{bmatrix} f_{j+1} \\ f_{j+2} \end{bmatrix}, \aleph = \begin{bmatrix} \aleph_1 \\ \aleph_2 \end{bmatrix}. \end{aligned} \tag{15}$$

Let

$$\hat{F} = (I-\upsilon)\,Y - h\,(\Gamma_1 F_1 + \Gamma_2 F_2) - \aleph = 0. \tag{16}$$

Applying the Newton iteration to (16) will generate the $(i+1)^{th}$ iterative y_{j+p} value as follows,

$$y_{j+p}^{(i+1)} = y_{j+p}^{(i)} - \frac{\hat{F}(y_{j+p}^{(i)})}{\hat{F}'(y_{j+p}^{(i)})},\; p = 1, 2. \tag{17}$$

Equation (17) is equivalent to

$$y_{j+p}^{(i+1)} - y_{j+p}^{(i)} = -\frac{(I-\upsilon)\,Y_{j+p}^{(i)} - h\,(\Gamma_1 F_1 + \Gamma_2 F_2) - \aleph}{(I-\upsilon) - h\left[\Gamma_1 \dfrac{\partial F_1}{\partial Y}\left(Y_{j+p}^{(i)}\right) + \Gamma_2 \dfrac{\partial F_2}{\partial Y}\left(Y_{j+p}^{(i)}\right)\right]}, \tag{18}$$

where

$$\frac{\partial F}{\partial Y}\left(Y_{j+p}^{(i)}\right)$$

denotes the Jacobian matrix of F with respect to Y.

4.1 Step Size Selection

The strategy of selecting the step size while implementing the adaptive step algorithm depends on the estimation of the local truncation error (LTE) and the prescribed tolerance limit (TOL). The LTE is obtained by computing the difference between the corrector formula for the y_{j+2} of consecutive orders given by

$$LTE = \left|y_{j+2}^{q} - y_{j+2}^{q-1}\right| \tag{19}$$

where q is the order of the derived method. The LTE for each step size ratio are presented in Table 5.

Table 5: Local truncation error for $\rho-$ASDIBBDF

r	Local truncation error
1	$LTE = -\frac{2\rho+3}{6\rho-19}y_{j-2} + \frac{3}{4}\frac{6\rho^2-\rho-15}{(6\rho-19)(\rho-2)}y_{j-1} - \frac{10\rho^2+\rho-21}{4(6\rho-19)(\rho-2)}y_{j+1} + \frac{3\rho(2\rho+3)}{2(6\rho-19)(\rho-2)}hf_{j+1} - \frac{3(2\rho+3)}{2(6\rho-19)(\rho-2)}hf_{j+2}$
2	$LTE = -\frac{2}{5}\frac{3\rho+4}{15\rho-34}y_{j-2} + \frac{2}{3}\frac{15\rho^2-\rho-28}{(15\rho-34)(3\rho-5)}y_{j-1} - \frac{8}{15}\frac{12\rho^2+\rho-20}{(15\rho-34)(3\rho-5)}y_{j+1} + \frac{4\rho(3\rho+4)}{(15\rho-34)(3\rho-5)}hf_{j+1} - \frac{4(3\rho+4)}{(15\rho-34)(3\rho-5)}hf_{j+2}$
$\frac{5}{8}$	$LTE = -\frac{112}{15}\frac{13\rho+21}{117\rho-461}y_{j-2} + \frac{1344}{65}\frac{117\rho^2-32\rho-357}{(117\rho-461)(13\rho-29)}y_{j-1} - \frac{112}{39}\frac{403\rho^2+40\rho-987}{(117\rho-461)(13\rho-29)}y_{j+1} + \frac{84\rho(13\rho+21)}{(117\rho-461)(13\rho-29)}hf_{j+1} - \frac{84(13\rho+21)}{(117\rho-461)(13\rho-29)}hf_{j+2}$

The strategies for selecting the step size are described based on the following conditions:

1. If (LTE $\leq$ TOL), then the step size is accepted and keep as constant i.e. considered the formula for $r = 1$. After a successful step, the following step increment is computed:

$$h_{new} = c \times h_{old} \times \left(\frac{TOL}{LTE}\right)^{\frac{1}{q}}$$

   where c is the safety factor and h_{old} is the step size from previous block. In our algorithm, we consider $c = 0.2$. If $h_{new} \geq \frac{8}{5} \times h_{old}$, then the new step size, h_{new} increase to $\frac{8}{5} \times h_{old}$ i.e considered the formula for $r = \frac{5}{8}$.

2. If (LTE $>$ TOL), then the step size is rejected and the step is repeated by halving the current step size and the new step size is computed as $h_{new} = \frac{1}{2} \times h_{old}$ i.e considered the formula for $r = 2$.

5 Numerical Experiments

In this section, the results for some numerical experiments to illustrate the performance of the derived method in Table 1 for TOL $= 10^{-i}, i = 2, 4, 6$ are presented. Three linear and nonlinear stiff initial value problems (IVPs) were selected and categorized into two cases.

In the first case, Problems 1 and 2 were tested with given theoretical solutions, where the maximum error, MAXE is evaluated as follows:

$$MAXE = \underbrace{max}_{1 \le s \le TS} \left(\underbrace{max}_{1 \le n \le EQN} \left| \frac{(y_s)_n - (y(t_s))_n}{M + N(y(t_s))_n} \right| \right), \tag{20}$$

with TS is the total steps, EQN is the number of equations in the system, $(y_s)_n$ and $(y(t_s))_n$ are the $n-$th component of approximate and theoretical solutions, respectively. The values $M = 1$ and $N = 1$ are set corresponds to a mixed error test for the algorithm.

In a situation where no theoretical solution to Problem 3 exists, the approximation values are obtained to be compared with MATLAB solver, ode15s at TOL $= 10^{-4}$.

We took three well-known test problems from the literature having no transient phase, which allows us to use adaptive step sizes, viz.:

Problem 1 The cosine problem presented in [20]:

$$y' = -2\pi \sin(2\pi x) - \frac{1}{\epsilon}\,(y - \cos(2\pi x))$$

where $\epsilon = 10^{-3}$, $y(0) = 1$ and $t \in [0, 10]$, with theoretical solution is $y(t) = \cos(2\pi x)$. The eigenvalues of the Jacobian matrix, λ is -1000. This cosine problem becomes increasingly stiff as $\epsilon \to 0$.

By demonstrating the effectiveness and efficiency of the proposed method, our goal is to make a substantial contribution to the field of numerical simulations for chemically reacting flows, specifically within the realms of applied and industrial mathematics, as exemplified through these two chemical reaction problems.

Problem 2 Nonlinear stiff chemical reaction problem (the Kaps problem) in [13]:

$$\begin{aligned} y_1' &= -\left(\epsilon^{-1} + 2\right) y_1 + \epsilon^{-1} {y_2}^2 \\ y_2' &= y_1 - y_2(1 + y_2) \end{aligned}$$

where $\epsilon = 10^{-5}$, $y_1(0) = 1, y_2(0) = 1$ and $t \in [0, 20]$, with theoretical solution is $y_1(t) = e^{-2t}, y_2(t) = e^{-t}$. The eigenvalues of the Jacobian matrix, λ are -1 and -100002 making the system highly stiff.

Problem 3 Nonlinear oregonator chemical reaction problem in [26]:

$$\begin{aligned} y_1' &= 77.27\left(y_2 - y_1 y_2 + y_1 - 8.375 \times 10^{-6} {y_1}^2\right) \\ y_2' &= \frac{1}{77.27}\,(y_3 - y_2 - y_1 y_2) \\ y_3' &= 0.161\,(y_1 - y_3) \end{aligned}$$

on the interval $t \in [0, 360]$ and with $y_1(0) = 1, y_2(0) = 2, y_3(0) = 3$. This is a well-known chemical model with a periodic solution describing the Belousov-Zhabotinskii reactions which exhibits a oscillatory behavior. The stiffness ratio could be as high as 3×10^4.

The comparison methods and abbreviations used in Tables 6–8 are described below:

TOL	Tolerance limit
MTD	Method
SS	Total of success steps
FS	Total of failure steps
TS	Total steps taken
MAXE	Maximum error
TIME	Computational time in seconds
$\rho-$ASDIBBDF	2$-$point $\rho-$Adaptive Step Diagonally Implicit BBDF
VSBBDF	2$-$point Variable Step Fully Implicit BBDF in [21]
VSSBBDF	2$-$point Variable Step Fully Implicit BBDF in [13]
ode15s	Variable order solver implemented in numerical differentiation formula

Table 6: Numerical results for Problem 1

TOL	MTD	SS	FS	TS	MAXE	TIME
10^{-2}	$\rho-$ASDIBBDF	53	0	53	5.08545E-5	4.45362E-5
	VSBBDF	87	19	106	6.18761E-5	9.87430E-4
	VSSBBDF	65	1	66	5.16437E-5	8.67844E-4
10^{-4}	$\rho-$ASDIBBDF	114	0	114	2.69909E-7	1.32737E-4
	VSBBDF	208	21	229	2.09325E-6	3.25709E-3
	VSSBBDF	116	0	116	1.54385E-6	1.49798E-3
10^{-6}	$\rho-$ASDIBBDF	396	0	396	1.51905E-8	7.21924E-4
	VSBBDF	580	37	617	5.05228E-8	8.55113E-3
	VSSBBDF	398	4	402	3.11839E-8	4.65798E-3

Table 7: Numerical results for Problem 2

TOL	MTD	SS	FS	TS	MAXE	TIME
10^{-2}	$\rho-$ASDIBBDF	26	0	26	3.50065E-5	6.28515E-4
	VSBBDF	45	0	45	6.48394E-4	4.00089E-3
	VSSBBDF	48	1	49	3.53673E-4	4.10795E-3
10^{-4}	$\rho-$ASDIBBDF	54	0	54	6.91081E-7	3.01038E-3
	VSBBDF	63	0	63	6.48780E-5	1.30311E-2
	VSSBBDF	70	4	74	1.59269E-5	1.63960E-2
10^{-6}	$\rho-$ASDIBBDF	102	0	102	4.91825E-9	9.42767E-3
	VSBBDF	99	0	99	6.48812E-6	3.98711E-2
	VSSBBDF	110	8	118	8.11971E-7	5.21691E-2

Table 8: Approximate solutions for Problem 3

	$y_1(t)$		$y_2(t)$		$y_3(t)$	
t	$\rho-$ASDIBBDF	ode15s	$\rho-$ASDIBBDF	ode15s	$\rho-$ASDIBBDF	ode15s
0	1	1	2	2	3	3
20	2.76058E+1	2.76940E+1	9.92734E-1	9.92435E-1	5.50050E+0	5.50457E+0
40	1.00058E+0	1.00057E+0	1.73568E+3	1.73516E+3	2.07151E+3	2.07106E+3
60	1.00075E+0	1.00087E+0	1.14456E+3	1.14423E+3	8.37285E+1	8.36955E+1
80	1.00144E+0	1.00145E+0	6.86466E+2	6.86263E+2	4.30660E+0	4.30685E+0
100	1.00244E+0	1.00244E+0	4.09248E+2	4.09127E+2	1.13415E+0	1.13405E+0
120	1.00411E+0	1.00411E+0	2.43882E+2	2.43810E+2	1.00881E+0	1.00880E+0
140	1.00689E+0	1.00692E+0	1.45331E+2	1.45292E+2	1.00616E+0	1.00618E+0
160	1.01165E+0	1.01176E+0	8.66045E+1	8.65971E+1	1.01004E+0	1.01007E+0
180	1.01974E+0	1.01976E+0	5.16080E+1	5.16073E+1	1.01696E+0	1.01693E+0
200	1.03360E+0	1.03362E+0	3.07530E+1	3.07528E+1	1.02883E+0	1.02884E+0
220	1.05771E+0	1.05778E+0	1.83247E+1	1.83272E+1	1.04937E+0	1.04931E+0
240	1.10082E+0	1.10078E+0	1.09175E+1	1.09201E+1	1.08581E+0	1.08586E+0
260	1.18173E+0	1.18173E+0	6.50156E+0	6.50320E+0	1.15320E+0	1.15318E+0
280	1.34885E+0	1.34878E+0	3.86561E+0	3.86663E+0	1.28841E+0	1.28833E+0
300	1.77972E+0	1.77907E+0	2.28185E+0	2.28291E+0	1.61375E+0	1.61331E+0
320	4.93887E+0	4.93348E+0	1.25096E+0	1.25143E+0	3.20493E+0	3.20311E+0
340	1.00056E+0	1.00056E+0	1.76765E+3	1.76788E+3	3.28356E+3	3.28917E+3
360	1.00081E+0	1.00081E+0	1.22876E+3	1.22859E+3	1.32463E+2	1.32369E+2
380	1.00135E+0	1.00135E+0	7.38859E+3	7.39127E+3	6.23734E+0	6.25253E+0
400	1.00227E+0	1.00227E+0	4.40577E+3	4.40733E+3	1.21118E+0	1.21162E+0

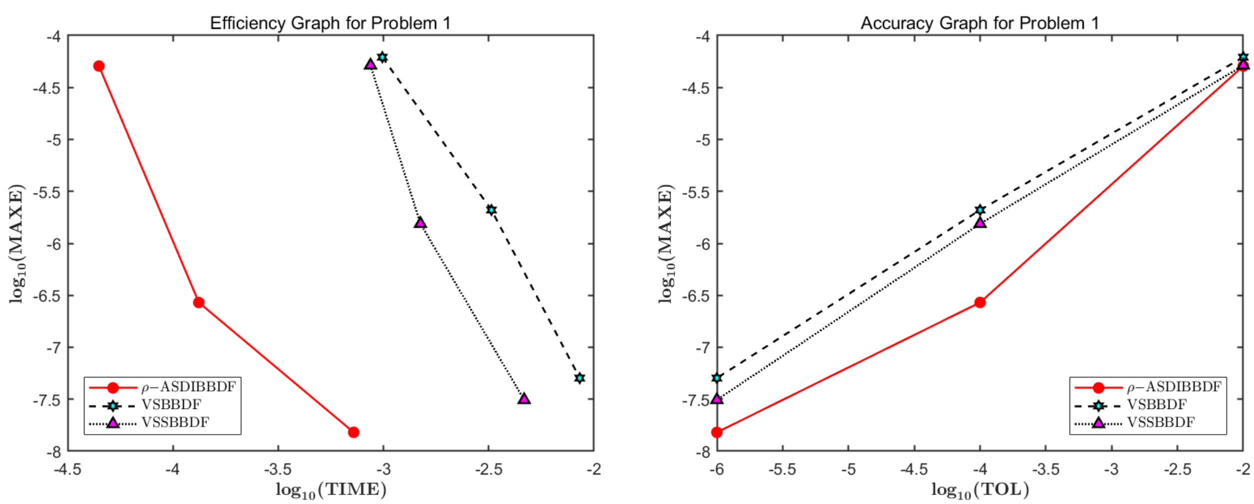


Figure 4: The accuracy and efficiency curves for Problem 1

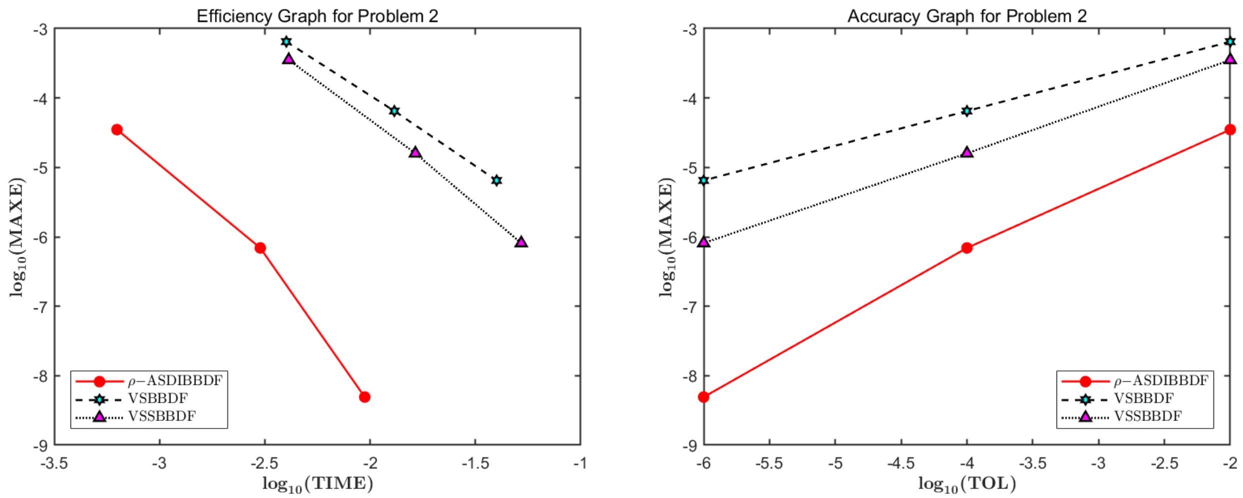


Figure 5: The accuracy and efficiency curves for Problem 2

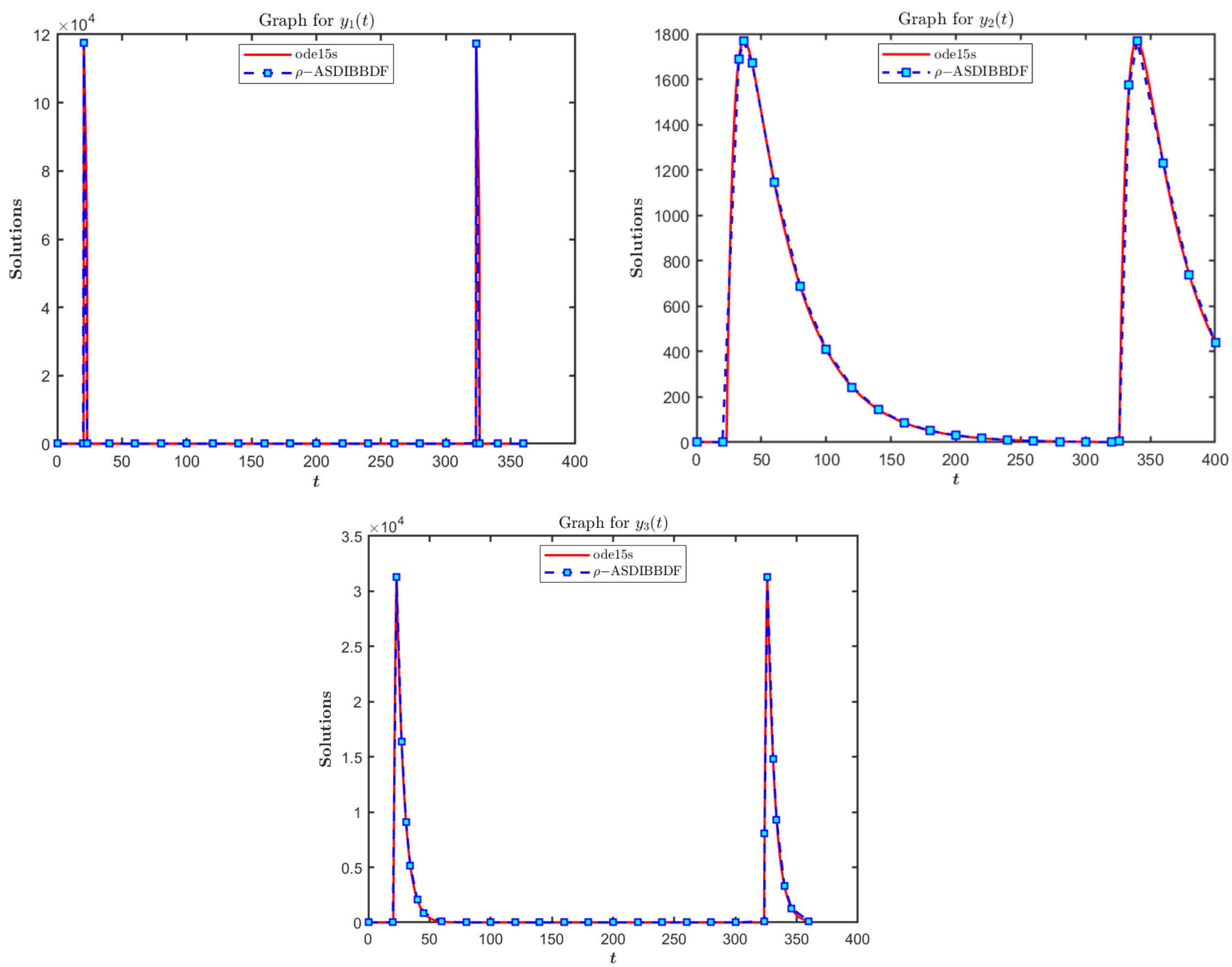


Figure 6: Graph profiles for Problem 3

Tables 6 and 7 present the numerical results of Problems 1 and 2, respectively. The $\rho-$ASDIBBDF exhibits impressive values of MAXE and TIME for each TOL when compared to VSBBDF and VSSBBDF. However, the results of Problem 1 exhibit a competitive MAXE when the TOL decreases, while still remaining within the specified tolerance limit. It can also be noted that the $\rho-$ASDIBBDF reaches the specified tolerance that indicates that the implemented algorithms have excellent performance.

When the MAXE are plotted against the TOL and TIME using logarithmic scales for both axes, all graphs in Figures 4$-$5 display a uniform-like error plotting, where the $\rho-$ASDIBBDF are in the lowest value of coordinate for a specific abscissa. As is evident from the performance graphs in Figures 4$-$5, it means the proposed method is stable in nature, accurate and efficient relative to the other methods of comparison.

From Table 8, it is indeed apparent that the approximations by the proposed method to the solutions of Problem 3 obtained by ode15s are very well agreed. The graph profiles in Figure 6 have proven the capability of the developed method on solving first order stiff IVPs arise in application systems of real-world problems in different level of stiffness.

6 Conclusion

Conclusively, this study presents an adaptive step 2$-$point $\rho-$type block method based on BDF in a diagonally implicit structure that is zero$-$stable, A_0-stable and $A(\alpha)-$stable. The relevant proof that the method satisfies the condition of the stability properties is also provided. The performance of the proposed method is excellent, as evidenced by the small maximum error recorded in the numerical results for the imposed tolerance. This experiment adds to a growing corpus of research showing that $\rho-$ASDIBBDF is significant in serving as an accurate numerical method and as an alternative solver for the physical systems of stiff ODEs. This underscores its potential applications across various industrial contexts.

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