A NEW FORMULAE OF VARIABLE STEP 3-POINT BLOCK BDF METHOD FOR SOLVING STIFF ODES

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Abstract

This paper derives a new variable step 3-point block method based on Backward Differentiation Formula (BDF) for solving stiff Ordinary Differential Equations (ODEs). The strategy involved in the developed method is to control the step

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size at each iteration to optimize the precision and produce three solution values simultaneously at each step. The method is analyzed in having the conditions for zero stability and found to be of order 6. The stability regions of the method are also investigated and presented in distinct graphs. The proposed method is compared to MATLAB’s suite ODEs solvers, namely, ode15s and ode23s. Numerical results obtained are provided to support the enhancement of the method in terms of accuracy.

1. Introduction

We consider block backward differentiation formula (BDF) for the solution of stiff first order ordinary differential equations (ODEs) of the form

\[ y' = f(x, y), \quad y(x_0) = y_0, \quad a \leq x \leq b. \]  

Implicit methods on solving stiff ODEs are known to perform better than explicit ones. Solving stiff ODEs using BDF method first was proposed by two chemist and their work can be found in [3]. Dahlquist [4] tried to solve stiff ODEs and explained the difficulties in differential equation solvers that may appear in integrating stiff problems. The implementation of the BDF methods for solving stiff ODEs was discussed by Gear [6] and he became one of the well-known researchers in the study of stiff ODEs. The order and the accuracy of BDF method for solving stiff ODEs were improved by Cash [2] through adding a future point, the method was called extended block BDF. Block implicit methods first were proposed by Milne [10] and his idea using a Runge-Kutta method later was extended by Rosser [12]. Convergence and stability properties of one-step implicit block method can be followed in [13, 16]. A class of block implicit method for solving stiff ODEs and \( A \)-stability properties can be seen in [17]. Block methods on solving stiff ODEs via backward differentiation formulae were developed in recent years and can be studied in [7]. Furthermore, variable step 2-point block BDF method for solving stiff ODEs can be followed in [8, 11, 14, 18]. A formulation of 3-point block BDF using variable step size of order 6 was obtained by [1] while the method did not deserve the condition for zero stability therefore the formulae can not be acceptable.
The aim of this paper is to introduce a new formula of variable step 3-point block backward differentiation formula to approximate three points concurrently at each iteration. In the following sections of this paper, the condition for zero stability and the analysis of the stability regions are illustrated. The numerical results obtained of the method are compared with stiff ODEs solvers in MATLAB defined as ode15s and ode23s. The advantage of the proposed method is that, the solutions are approximated at more than one point simultaneously to improve the accuracy of the method.

2. Derivation of Variable Step 3-Point Block BDF Method

In a 3-point block BDF method, three solution values \( y_{n+1}, y_{n+2}, \) and \( y_{n+3} \), with step size \( h \) are computed simultaneously in a block using four back values \( y_{n-3}, y_{n-2}, y_{n-1}, \) and \( y_n \), with step size \( rh \) (Figure 1).

\[
\begin{bmatrix}
-\frac{h}{3} & \frac{h}{3} & \frac{h}{3} & \frac{h}{3} & \frac{h}{3} \\
-\frac{r}{3} & 1 & \frac{r}{3} & 0 & \frac{r}{3} \\
-\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \\
-\frac{1}{3} & \frac{1}{3} & -\frac{1}{3} & \frac{1}{3} & \frac{1}{3}
\end{bmatrix}
\]

\[y_{n-3} \hspace{1cm} y_{n-2} \hspace{1cm} y_{n-1} \hspace{1cm} y_n \hspace{1cm} y_{n+1} \hspace{1cm} y_{n+2} \hspace{1cm} y_{n+3}\]

**Figure 1.** Interpolation points involved in the 3-point variable step BBDF.

In above figure, \( r \) is the step ratio in a block. We limit the amount of step size increase to ensure zero stability. In this case, we consider \( r = 1, 2, \) and \( \frac{1000}{1196} \), which corresponds to constant step size, halving and increasing the step size by a factor of 1.196. The motivation behind the choice of each value of \( r \) are as follows; first is to optimize the total number of steps and the second is that each value used ensures a zero stable formula. The interpolating polynomial \( P_k(x) \) of degree \( k \), which interpolates the points \( (x_{n-3}, y_{n-3}), (x_{n-2}, y_{n-2}), \ldots, (x_{n+3}, y_{n+3}) \) is defined as

\[
P_k(x) = \sum_{j=0}^{k} L_{k,j}(x)y(x_{n+3-j}), \tag{2}
\]
where

\[
L_{k,j}(x) = \prod_{i=0}^{\infty} \frac{x - x_{n+3-i}}{x_{n+3-j} - x_{n+3-i}} \quad \text{for } j = 0, 1, \ldots, k \ (k = 6),
\]

the associated polynomial for (2) can be written as

\[
P(x) =
\]

\[
(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n})(x - x_{n+1})(x - x_{n+2})
\]

\[
(x_{n+3} - x_{n-3})(x_{n+3} - x_{n-2})(x_{n+3} - x_{n-1})(x_{n+3} - x_{n})(x_{n+3} - x_{n+1})(x_{n+3} - x_{n+2}) y_{n+3}
\]

\[
+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n})(x - x_{n+1})(x - x_{n+3})}{(x_{n+2} - x_{n-3})(x_{n+2} - x_{n-2})(x_{n+2} - x_{n-1})(x_{n+2} - x_{n})(x_{n+2} - x_{n+1})(x_{n+2} - x_{n+3})} y_{n+2}
\]

\[
+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n})(x - x_{n+1})(x - x_{n+3})}{(x_{n+1} - x_{n-3})(x_{n+1} - x_{n-2})(x_{n+1} - x_{n-1})(x_{n+1} - x_{n})(x_{n+1} - x_{n+1})(x_{n+1} - x_{n+3})} y_{n+1}
\]

\[
+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n})(x - x_{n+1})(x - x_{n+3})}{(x_{n} - x_{n-3})(x_{n} - x_{n-2})(x_{n} - x_{n-1})(x_{n} - x_{n+1})(x_{n} - x_{n+1})(x_{n} - x_{n+3})} y_{n}
\]

\[
+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n})(x - x_{n+1})(x - x_{n+3})}{(x_{n-1} - x_{n-3})(x_{n-1} - x_{n-2})(x_{n-1} - x_{n-1})(x_{n-1} - x_{n})(x_{n-1} - x_{n+1})(x_{n-1} - x_{n+3})} y_{n-1}
\]

\[
+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n})(x - x_{n+1})(x - x_{n+3})}{(x_{n-2} - x_{n-3})(x_{n-2} - x_{n-1})(x_{n-2} - x_{n})(x_{n-2} - x_{n+1})(x_{n-2} - x_{n+1})(x_{n-2} - x_{n+3})} y_{n-2}
\]

\[
+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n})(x - x_{n+1})(x - x_{n+3})}{(x_{n-3} - x_{n-3})(x_{n-3} - x_{n-1})(x_{n-3} - x_{n})(x_{n-3} - x_{n+1})(x_{n-3} - x_{n+2})(x_{n-3} - x_{n+3})} y_{n-3}.
\]

(3)

Define \( s = \frac{x - x_{n+1}}{h} \) and replace \( x = x_{n+1} + sh \) in (3), gives

\[
p(x) = p(x_{n+1} + sh)
\]

\[
= \frac{(s + 1 + 3r)(s + 1 + 2r)(s + 1 + r)(s + 1)s(s - 1)}{6(3 + 3r)(3 + 2r)(3 + r)} y_{n+3}
\]

\[
+ \frac{(s + 1 + 3r)(s + 1 + 2r)(s + 1 + r)(s + 1)s(s - 2)}{(- 2)(2 + 3r)(2 + 2r)(2 + r)} y_{n+2}
\]

\[
+ \frac{(s + 1 + 3r)(s + 1 + 2r)(s + 1 + r)(s + 1)s(s - 2)}{2(1 + 3r)(1 + 2r)(1 + r)} y_{n+1}
\]
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\[ + \frac{(s + 1 + 3r)(s + 1 + 2r)(s + 1 + r)s(s - 1)(s - 2)}{(-36)r^3} y_n \]

\[ + \frac{(s + 1 + 3r)(s + 1 + 2r)(s + 1)s(s - 1)(s - 2)}{2r^3(-1 - r)(2 + r)(-3 - r)} y_{n-1} \]

\[ + \frac{(s + 1 + 3r)(s + 1 + r)(s + 1)s(s - 1)(s - 2)}{2r^3(1 + 2r)(-2 - 2r)(3 + 2r)} y_{n-2} \]

\[ + \frac{(s + 1 + 2r)(s + 1 + r)(s + 1)s(s - 1)(s - 2)}{(-6)r^3(1 + 3r)(-2 - 3r)(3 + 3r)} y_{n-3}. \] (4)

Differentiating (4) with respect to \( s \) and substituting \( s = 0, 1, \) and 2 gives

\[ h f_{n+1} = \frac{-(6r^2 + 5r + 1)}{18(r + 3)(2r + 3)} y_{n+3} + \frac{6r^2 + 5r + 1}{2(r + 2)(3r + 2)} y_{n+2} \]

\[ + \frac{-(6r^3 - 11r^2 - 18r - 5)}{2(r + 1)(2r + 1)(3r + 1)} y_{n+1} + \frac{-(6r^3 + 11r^2 + 6r + 1)}{18r^3} y_{n} \]

\[ + \frac{6r^2 + 5r + 1}{r^3(r + 1)(r + 2)(r + 3)} y_{n-1} + \frac{-(3r + 1)}{2r^3(2r + 1)(2r + 3)} y_{n-2} \]

\[ + \frac{2r + 1}{9r^3(3r + 1)(3r + 2)} y_{n-3}; \] (5)

\[ h f_{n+2} = \frac{2(3r^2 + 8r + 4)}{9(r + 3)(2r + 3)} y_{n+3} + \frac{3r^3 + 22r^2 + 36r + 16}{2(r + 1)(r + 2)(3r + 2)} y_{n+2} \]

\[ + \frac{-(2)(3r^2 + 8r + 4)}{(2r + 1)(3r + 1)} y_{n+1} + \frac{3r^3 + 11r^2 + 12r + 4}{18r^3} y_{n} \]

\[ + \frac{-(2)(3r + 2)}{r^3(r + 2)(r + 3)} y_{n-1} + \frac{3r^2 + 8r + 4}{2r^3(r + 1)(2r + 1)(2r + 3)} y_{n-2} \]

\[ + \frac{(-2)(r + 2)}{9r^3(3r + 1)(3r + 2)} y_{n-3}; \] (6)
Replacing $r = 1$, 2, and $\frac{1000}{1196}$ into (5), (6), and (7), respectively, gives the coefficients of the method as given below, which are stored in the codes. The values of $r$ chosen ensure the zero stability of the method.

For $r = 1$,

\[ y_{n+1} = -\frac{1}{35} y_{n-3} + \frac{8}{35} y_{n-2} - \frac{6}{7} y_{n-1} + \frac{16}{7} y_n - \frac{24}{35} y_{n+1} + \frac{2}{35} y_{n+3} + \frac{12}{7} \frac{h f_{n+1}}{}, \]

\[ y_{n+2} = \frac{2}{77} y_{n-3} - \frac{15}{77} y_{n-2} + \frac{50}{77} y_{n-1} - \frac{100}{77} y_n + \frac{150}{77} y_{n+1} - \frac{10}{77} y_{n+3} + \frac{60}{77} \frac{h f_{n+2}}{}, \]

\[ y_{n+3} = -\frac{10}{147} y_{n-3} + \frac{24}{49} y_{n-2} - \frac{75}{49} y_{n-1} + \frac{400}{147} y_n - \frac{150}{49} y_{n+1} + \frac{120}{49} y_{n+2} + \frac{20}{49} \frac{h f_{n+3}}{}, \] (8)

For $r = 2$,

\[ y_{n+1} = -\frac{25}{3552} y_{n-3} + \frac{21}{296} y_{n-2} - \frac{245}{592} y_{n-1} + \frac{1225}{296} y_n - \frac{3675}{1184} y_{n+2} + \frac{35}{111} y_{n+3} + \frac{210}{37} \frac{h f_{n+1}}{}, \]

\[ y_{n+2} = \frac{1}{325} y_{n-3} - \frac{16}{875} y_{n-2} + \frac{12}{125} y_{n-1} - \frac{16}{25} y_n + \frac{1536}{875} y_{n+1} - \frac{512}{2652} y_{n+3} + \frac{24}{25} \frac{h f_{n+2}}{}, \]
\[ y_{n+3} = -\frac{175}{46112} y_{n-3} + \frac{405}{11528} y_{n-2} - \frac{3969}{23056} y_{n-1} + \frac{11025}{11528} y_n - \frac{2835}{1441} y_{n+1} \]
\[ + \frac{99225}{46112} y_{n+2} + \frac{630}{1441} h f_{n+3}. \]  

For \( r = \frac{1000}{1196} \),
\[ y_{n+1} = -\frac{311249130548929261}{682184355671875000000} y_{n-3} + \frac{4828453731348401349}{14139637164296875000000} y_{n-2} \]
\[ - \frac{5614735319756923077601}{49223346190681250000000} y_{n-1} + \frac{23525925314746689}{10121429609375000000000} y_n \]
\[ + \frac{385670907241749}{740470187020480} y_{n+2} + \frac{42852323026861}{1037962484956705} y_{n+3} \]
\[ + \frac{920289798}{647771495} h f_{n+1}, \]
\[ y_{n+2} = \frac{21912216496200784}{432892639115234375} y_{n-3} - \frac{163183509197182087744}{460625417024158203125} y_{n-2} \]
\[ + \frac{498329846860832181}{47334468126953125} y_{n-1} - \frac{683744261438016}{412671724609375} y_n \]
\[ + \frac{358685514196992}{177091183950373} y_{n+1} - \frac{39853946021888}{338559105010357} y_{n+3} \]
\[ + \frac{156891024}{211287923} h f_{n+2}, \]
\[ y_{n+3} = -\frac{20521277884988304247681}{14516633027539409375000000} y_{n-3} + \frac{155864674783310403807}{164050399688328125000000} y_{n-2} \]
\[ - \frac{231213758866944231807}{87055531248875000000000} y_{n-1} + \frac{773863453129498281}{205319649171875000000} y_n \]
\[ + \frac{3805885835630163}{11013687633475597} y_{n+1} + \frac{3805885835630163}{15020909583805888} y_{n+2} \]
\[ + \frac{5278170546}{13140457547} h f_{n+3}. \]  

(10)
3. Order of the Method

This section derives the order of the method corresponding to the equations in (8), (9), and (10). First, we consider the method (8) while \( r = 1 \). It can be rewritten as

\[
\begin{align*}
&+ \frac{1}{35} y_{n-3} - \frac{8}{35} y_{n-2} + \frac{6}{7} y_{n-1} - \frac{16}{7} y_n + \frac{24}{35} y_{n+1} - \frac{2}{35} y_{n+2} - \frac{2}{7} y_{n+3} = \frac{12}{7} hf_{n+1}, \\
&- \frac{2}{77} y_{n-3} + \frac{15}{77} y_{n-2} - \frac{50}{77} y_{n-1} + \frac{100}{77} y_n - \frac{150}{77} y_{n+1} + y_{n+2} + \frac{10}{77} y_{n+3} = \frac{60}{77} hf_{n+2}, \\
&+ \frac{10}{147} y_{n-3} - \frac{24}{49} y_{n-2} + \frac{75}{49} y_{n-1} - \frac{400}{147} y_n + \frac{150}{49} y_{n+1} - \frac{120}{49} y_{n+2} + y_{n+3} = \frac{20}{49} hf_{n+3}. \quad (11)
\end{align*}
\]

The matrix form of (11) is associated with

\[
\begin{bmatrix}
0 & 0 & \frac{1}{35} & y_{n-5} \\
0 & 0 & -\frac{2}{77} & y_{n-4} \\
0 & 0 & \frac{10}{147} & y_{n-3} \\
\end{bmatrix} + \begin{bmatrix}
\frac{8}{35} & \frac{6}{7} & -\frac{16}{7} \\
15 & -\frac{50}{77} & \frac{100}{77} \\
-\frac{24}{49} & \frac{75}{49} & -\frac{400}{147} \\
\end{bmatrix} \begin{bmatrix}
y_{n-2} \\
y_{n-1} \\
y_n \\
\end{bmatrix} = \begin{bmatrix}
\frac{12}{7} & 0 & 0 \\
0 & \frac{60}{77} & 0 \\
0 & 0 & \frac{20}{49} \\
\end{bmatrix} \begin{bmatrix}
f_{n+1} \\
f_{n+2} \\
f_{n+3} \\
\end{bmatrix}. \quad (12)
\]

Let

\[
\alpha_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \alpha_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \alpha_2 = \begin{bmatrix} 1 \\ \frac{2}{77} \\ \frac{10}{147} \end{bmatrix}, \quad \alpha_3 = \begin{bmatrix} -\frac{8}{35} \\ 15 \\ -\frac{24}{49} \end{bmatrix}, \quad \alpha_4 = \begin{bmatrix} \frac{6}{7} \\ \frac{50}{77} \\ \frac{75}{49} \end{bmatrix}.
\]
\[ \alpha_5 = \begin{bmatrix} \frac{16}{7} \\ \frac{100}{77} \\ -\frac{400}{147} \end{bmatrix}, \quad \alpha_6 = \begin{bmatrix} 1 \\ -\frac{150}{77} \\ \frac{150}{49} \end{bmatrix}, \quad \alpha_7 = \begin{bmatrix} \frac{24}{35} \\ -\frac{120}{49} \end{bmatrix}, \quad \alpha_8 = \begin{bmatrix} \frac{2}{35} \\ \frac{10}{77} \end{bmatrix}, \]

\[ \beta_6 = \begin{bmatrix} \frac{12}{7} \\ 0 \\ 0 \end{bmatrix}, \quad \beta_7 = \begin{bmatrix} 0 \\ \frac{60}{77} \end{bmatrix}, \quad \beta_8 = \begin{bmatrix} 0 \\ \frac{20}{49} \end{bmatrix}. \]

The linear difference operator \( L \) is defined by

\[ L[y(x), h] = \sum_{j=0}^{8} [\alpha_j y(x + jh) - h\beta_j y'(x + jh)]. \quad (13) \]

Expanding the function \( y(x + jh) \) and its derivative \( y'(x + jh) \) as Taylor series around \( x \) and substituting in (13) leads to

\[ L[y(x); h] = C_0 y(x) + C_1 h y^{(1)}(x) + C_2 h^2 y^{(2)}(x) + \cdots + C_q h^q y^{(q)}(x) + \cdots, \quad (14) \]

where \( C_q \) are constants. The difference operator (13) and the associated method (11) is considered of order \( p \) if \( c_0 = c_1 = \cdots = c_p = 0 \) and \( c_{p+1} \neq 0 \). In this case,

\[ c_0 = \sum_{j=0}^{8} \alpha_j = 0, \]

\[ c_1 = \sum_{j=0}^{8} (j\alpha_j) - \sum_{j=0}^{8} \beta_j = 0, \]

\[ c_2 = \sum_{j=0}^{8} \frac{(j^2\alpha_j)}{2!} - \sum_{j=0}^{8} (j\beta_j) = 0, \]
\[
\begin{align*}
c_5 &= \sum_{j=0}^{8} \left( \frac{8^j \alpha_j}{5!} \right) - \sum_{j=0}^{8} \left( \frac{8^j \beta_j}{4!} \right) = 0, \\
c_6 &= \sum_{j=0}^{8} \left( \frac{8^j \alpha_j}{6!} \right) - \sum_{j=0}^{8} \left( \frac{8^j \beta_j}{5!} \right) = 0, \\
c_7 &= \sum_{j=0}^{8} \left( \frac{8^j \alpha_j}{7!} \right) - \sum_{j=0}^{8} \left( \frac{8^j \beta_j}{6!} \right) = \begin{bmatrix}
-\frac{4}{245} \\
\frac{10}{539} \\
\frac{20}{343}
\end{bmatrix} \neq \begin{bmatrix}
0 \\
0 \\
0
\end{bmatrix}.
\end{align*}
\]

Therefore, the order of the method (8) is 6 and the error constant is determined by

\[
c_7 = \begin{bmatrix}
-\frac{4}{245} \\
\frac{10}{539} \\
\frac{20}{343}
\end{bmatrix}.
\]

Applying a similar procedure to the method (9) and (10) shows that the order of them is 6.

4. Stability of the 3-Point Block BDF Method

In this section, we discuss about the conditions for the stability of the method in (8), (9), and (10). We start by the following definitions:

**Definition 1** ([9]). A method is said to be zero stable if all the roots of first characteristic polynomial have modulus less than or equal to unity and those of modulus unity are simple.

**Definition 2** ([9]). A method is said to be absolutely stable in a region \( R \) for a given \( h\lambda \) if for that \( h\lambda \), all the roots \( r_s \) of stability polynomial \( \pi(r, h\lambda) = \rho(r) - h\lambda\sigma(r) = 0 \) satisfy \(|r_s| < 1, s = 1, 2, ..., k\).
**Definition 3** ([5]). A method is said to be \( A \)-stable if the stability region covers the entire negative left half plane.

The stability regions of the method are determined by substituting linear test problem

\[
y' = \lambda y \quad (\lambda < 0, \ \lambda \ \text{complex}),
\]

into Equations (8), (9), and (10). We obtain the following form:

\[
AY_m = BY_{m-1} + CY_{m-2},
\]

where \( A, B, \) and \( C \) are the matrix coefficients and can be specified based on the coefficients in (8), (9), and (10), respectively.

We define \( n = mr \), where \( m \) is the block number and \( r \) is the number of points in the block. Here, \( r = 3 \) and \( n = 3m \). Hence,

\[
Y_m = \begin{bmatrix}
  y_{3m+1} \\ y_{3m+2} \\ y_{3m+3}
\end{bmatrix} = \begin{bmatrix}
  y_{n+1} \\ y_{n+2} \\ y_{n+3}
\end{bmatrix} ; \quad Y_{m-1} = \begin{bmatrix}
  y_{3(m-1)+1} \\ y_{3(m-1)+2} \\ y_{3(m-1)+3}
\end{bmatrix} = \begin{bmatrix}
  y_{n-2} \\ y_{n-1} \\ y_{n}
\end{bmatrix} ;
\]

and

\[
Y_{m-2} = \begin{bmatrix}
  y_{3(m-2)+1} \\ y_{3(m-2)+2} \\ y_{3(m-2)+3}
\end{bmatrix} = \begin{bmatrix}
  y_{n-5} \\ y_{n-4} \\ y_{n-3}
\end{bmatrix} .
\]

The stability polynomial of the method, \( R(t, \hat{h}) \), where \( \hat{h} = h\lambda \) is defined by

\[
\det(At^2 - Bt - C),
\]

while the absolute stability region of the method is determined by solving \( \det(At^2 - Bt - C) = 0 \) in the \( h\lambda \) plane. The following gives the absolute stability regions of the method for the chosen step sizes, \( r = 1, 2, \) and \( \frac{1000}{1196} \), respectively,
(i) \[ R(t, \hat{h}) = -\frac{1}{79233} t^2 + \frac{40}{2401} t^3 + \frac{232}{26411} t^3 \hat{h} + \frac{1852}{2401} t^4 \hat{h} + \frac{20640}{26411} t^4 \hat{h}^2 \]
\[ + \frac{2400}{26411} t^4 \hat{h}^2 - \frac{286568}{79233} t^5 \hat{h} - \frac{72216}{26411} t^5 \hat{h}^2 - \frac{109920}{26411} t^5 \hat{h}^2 \]
\[ + \frac{10673}{3773} t^6 - \frac{109036}{26411} t^6 \hat{h} + \frac{8880}{3773} t^6 \hat{h}^2 - \frac{14400}{26411} t^6 \hat{h}^3 \]
\[ = 0; \quad (16) \]

(ii) \[ R(t, \hat{h}) = -\frac{1}{42653600} t^2 + \frac{22257}{42653600} t^3 + \frac{243}{1066340} t^3 \hat{h} + \frac{359023}{1332925} t^4 \hat{h} \]
\[ + \frac{2029923}{10663400} t^4 \hat{h}^2 + \frac{2205}{106634} t^4 \hat{h}^2 - \frac{157887}{20350} t^5 \hat{h} - \frac{11586078}{1332925} t^5 \hat{h} \]
\[ - \frac{1460592}{266585} t^5 \hat{h}^2 + \frac{1996367}{266585} t^6 - \frac{1506528}{121175} t^6 \hat{h} + \frac{202365}{24235} t^6 \hat{h}^2 \]
\[ - \frac{127008}{53317} t^6 \hat{h}^3 \]
\[ = 0; \quad (17) \]

(iii) \[ R(t, \hat{h}) = -\frac{136479626362672279183343141245755554499}{219541714200576769268330944213867187500000} t^2 \]
\[ + \frac{9490509363205766214390132478878357434499}{21954171420057676926833094421386718750000} t^3 \hat{h} \]
\[ + \frac{556974234307066011541528846992927579}{23109654126376502028245362548828125000} t^3 \hat{h} \]
\[ + \frac{24804016848454261960506657711429351187}{219541714200576769268330944213867187500} t^4 \hat{h} \]
\[ + \frac{115028677210765616692778596732358021703}{87816685680230707707332377685546875000} t^4 \hat{h} \]
\[ + \frac{280130327026383263162046362322}{1878431779256271826167353515625} t^4 \hat{h}^2 \]
\[ - \frac{51549616346769672572149818076542327}{1405066970883691323317318042968750} t^5 \hat{h} \]
\[ - \frac{1297010472298974226423732248769653}{70253348544184561658659021484375} t^5 \hat{h} \]
\[ = 0; \quad (17) \]
For zero stability, we set \( \hat{h} = 0 \) in (16), (17), and (18) to obtain the first characteristic polynomial as

\[
(i) \quad \frac{10673}{3773} t^6 - \frac{286568}{79233} t^5 + \frac{1852}{2401} t^4 + \frac{40}{2401} t^3 - \frac{1}{79233} t^2 = 0; \quad (19)
\]

\[
(ii) \quad \frac{1996376}{266585} t^6 - \frac{157887}{20350} t^5 + \frac{359023}{1332925} t^4 + \frac{22257}{42653600} t^3 - \frac{1}{42653600} t^2 = 0; \quad (20)
\]

\[
(iii) \quad + \frac{922666265893348903771816}{369678463048535435528503} t^6
\]

\[
- \frac{5154961634679672572149818076542327}{140506697083691323317318042968750} t^5
\]

\[
+ \frac{2480401684845261960506657711429351187}{21954171420057676926833094421386718750} t^4
\]

\[
+ \frac{9490509363205766214390132478878357434499}{21954171420057676926833094421386718750000} t^3
\]

\[
- \frac{13647962636267227918343141245775554499}{219541714200576769268330944213867187500000} t^2
\]

\[= 0. \quad (21)\]
The roots obtained from (19), (20), and (21) are listed below, respectively,

(i) \( t = -0.02041446823, t = 0, t = 0, t = 0.0007327983430, \)
\( t = 0.2982439521, t = 1; \)

(ii) \( t = -0.001881407546, t = 0, t = 0, t = 0.00004393458062, \)
\( t = 0.03787462228, t = 1; \)

(iii) \( t = -0.03559407865, t = 0, t = 0, t = 0.001387943697, \)
\( t = 0.5041742684, t = 1. \)

As all the roots have modulus less than or equal to unity, so the method is zero stable when \( r = 1, 2, \) and \( \frac{1000}{1196}. \) The stability regions of the method when \( r = 1, 2, \) and \( \frac{1000}{1196} \) are shown in Figures 2, 3, and 4.

**Figure 2.** Stability region when \( r = 1. \)
Figure 3. Stability region when $r = 2$.

Figure 4. Stability region when $r = \frac{1000}{1196}$.
The stability region while $r = 2$ in Figure 3 covers the whole negative left half plane, so the method is considered as $A$-stable. The stability regions when $r = 1$ and $r = \frac{1000}{1196}$, which are shown in Figure 2 and Figure 4, respectively, almost cover the entire negative left half plane, hence the method is stiffly stable.

To obtain $r = \frac{1000}{1196}$, different values of $r$ have been tested. Zero stability and absolute stability of the method for the $r$ tested are listed in Table 1.

**Table 1. The values of $r$ tested for the 3-point**

<table>
<thead>
<tr>
<th>$r$</th>
<th>$\frac{1}{r}$</th>
<th>Status of the method</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{2}$</td>
<td>2</td>
<td>not zero stable</td>
</tr>
<tr>
<td>$r = \frac{10}{19}$</td>
<td>1.9</td>
<td>not zero stable</td>
</tr>
<tr>
<td>$r = \frac{5}{8}$</td>
<td>1.6</td>
<td>not zero stable</td>
</tr>
<tr>
<td>$r = \frac{2}{3}$</td>
<td>1.5</td>
<td>zero stable not absolutely stable</td>
</tr>
<tr>
<td>$r = \frac{5}{7}$</td>
<td>1.4</td>
<td>zero stable not absolutely stable</td>
</tr>
<tr>
<td>$r = \frac{10}{13}$</td>
<td>1.3</td>
<td>zero stable not absolutely stable</td>
</tr>
<tr>
<td>$r = \frac{5}{6}$</td>
<td>1.2</td>
<td>zero stable not absolutely stable</td>
</tr>
<tr>
<td>$r = \frac{1000}{1198}$</td>
<td>1.1198</td>
<td>zero stable not absolutely stable</td>
</tr>
<tr>
<td>$r = \frac{1000}{1197}$</td>
<td>1.1197</td>
<td>zero stable not absolutely stable</td>
</tr>
<tr>
<td>$r = \frac{1000}{1196}$</td>
<td>1.1196</td>
<td>zero stable and absolutely stable</td>
</tr>
</tbody>
</table>
From Table 1, it is seen that when \( r = \frac{1}{2}, \frac{10}{19}, \) and \( \frac{5}{8} \) the method is not zero stable as it does not satisfy the Definition 1. Therefore, the 3-point block BDF of variable step size formulated by \([1]\), is not acceptable as the method is not zero stable when \( r = \frac{1}{2} \). Choosing 

\[
\frac{2}{3} \cdot \frac{5}{7} \cdot \frac{10}{13} \cdot \frac{5}{6} \cdot \frac{1000}{1198}, \text{ and } \frac{1000}{1197}
\]

gives a zero stable method not absolutely stable. For example, if we set \( \hat{h} = 3.00 \) in the stability polynomials obtained for \( r = \frac{1000}{1197} \) and solve it for \( t \), it gives at least one root bigger than one. Therefore, by the Definition 2, the method is not absolutely stable for \( r = \frac{1000}{1197} \). Setting different amount of \( \hat{h} \) for 

\[
\frac{1000}{1198}, \frac{5}{6} \cdot \frac{10}{13} \cdot \frac{5}{7}, \text{ and } \frac{2}{3}
\]

gives a similar results, which shows that the method is not absolutely stable in the \( r \) chosen.

Figures 5-10 are provided to show the stability regions when 

\[
\frac{1000}{1197}, \frac{1000}{1198}, \frac{5}{6} \cdot \frac{10}{13} \cdot \frac{5}{7}, \text{ and } \frac{2}{3}.
\]
Figure 5. Stability region when \( r = \frac{1000}{1197} \).

Figure 6. Stability region when \( r = \frac{1000}{1198} \).
Figure 7. Stability region when \( r = \frac{5}{6} \).

Figure 8. Stability region when \( r = \frac{10}{13} \).
Figure 9. Stability region when $r = \frac{5}{7}$.

Figure 10. Stability region when $r = \frac{2}{3}$.
5. Implementation of the 3-Point Block BDF Method

Newton’s iteration is applied for the implementation of the method. First, we define the error in the \((i)\)th iteration as

\[
\text{error}^{(i)} = |y_{\text{exact}}^{(i)} - y_{\text{approximate}}^{(i)}|,
\]

and the maximum error is given by

\[
\text{MAXE} = \max_{1 \leq i \leq \text{TNS}} (\text{error}^{(i)}).
\]

The abbreviation TNS gives the total number of steps.

Let \(y_{n+j}^{(i+1)}\) denote the \((i+1)\)th iterative values of \(y_{n+j}\), define

\[
e_{n+j}^{(i+1)} = y_{n+j}^{(i+1)} - y_{n+j}^{(i)}, \quad j = 1, 2, 3.
\]

The 3-point block BDF method can be written as

\[
\begin{align*}
y_{n+1} &= \alpha_1 h f_{n+1} + \beta_1 y_{n+2} + \gamma_1 y_{n+3} + \eta_1, \\
y_{n+2} &= \alpha_2 h f_{n+2} + \beta_2 y_{n+1} + \gamma_2 y_{n+3} + \eta_2, \\
y_{n+3} &= \alpha_3 h f_{n+3} + \beta_3 y_{n+1} + \gamma_3 y_{n+2} + \eta_3,
\end{align*}
\]

where \(\alpha_i, \beta_i,\) and \(\gamma_i, \, i = 1, 2, 3\) represent the coefficients when \(r = 1, 2,\) and \(\frac{1000}{1196}\), respectively. \(\eta_1, \eta_2\) and \(\eta_3\) represent the back values. Let

\[
\begin{align*}
F_1 &= y_{n+1} - \beta_1 y_{n+2} - \gamma_1 y_{n+3} - \alpha_1 h f_{n+1} - \eta_1, \\
F_2 &= -\beta_2 y_{n+1} + y_{n+2} - \gamma_2 y_{n+3} - \alpha_2 h f_{n+2} - \eta_2, \\
F_3 &= -\beta_3 y_{n+1} - \gamma_3 y_{n+2} + y_{n+3} - \alpha_3 h f_{n+3} - \eta_3.
\end{align*}
\]

Newton’s iteration is defined as

\[
y_{n+j}^{(i+1)} = y_{n+j}^{(i)} - \frac{\partial F_j^{(i)}}{\partial y_{n+j}^{(i)}} F_j^{(i)}, \quad j = 1, 2, 3.
\]
Hence, Newton’s iteration can be defined in the form

\[
\begin{bmatrix}
    y_n^{(i+1)} \\
y_{n+1}^{(i+1)} \\
y_{n+2}^{(i+1)} \\
y_{n+3}^{(i+1)}
\end{bmatrix}
= \begin{bmatrix}
y_{n+1}^{(i)} \\
y_{n+2}^{(i)} \\
y_{n+3}^{(i)} \\
y_{n+4}^{(i)}
\end{bmatrix}
\begin{bmatrix}
    \partial F_1^{(i)} \\
    \partial F_2^{(i)} \\
    \partial F_3^{(i)} \\
    \partial F_4^{(i)}
\end{bmatrix}^{-1}
\begin{bmatrix}
    F_1^{(i)} \\
    F_2^{(i)} \\
    F_3^{(i)} \\
    F_4^{(i)}
\end{bmatrix}.
\]  

(24)

Equation (24) is equivalent to

\[
\begin{bmatrix}
    \partial F_1^{(i)} \\
    \partial F_2^{(i)} \\
    \partial F_3^{(i)} \\
    \partial F_4^{(i)}
\end{bmatrix}
\begin{bmatrix}
    e_{n+1}^{(i+1)} \\
    e_{n+2}^{(i+1)} \\
    e_{n+3}^{(i+1)}
\end{bmatrix}
= \begin{bmatrix}
    F_1^{(i)} \\
    F_2^{(i)} \\
    F_3^{(i)} \\
    F_4^{(i)}
\end{bmatrix}.
\]  

(25)

Let \( J \) denote the Jacobian matrix in (25), then

\[
J = \begin{bmatrix}
    1 - \alpha_1 h \frac{\partial f_{n+1}^{(i)}}{\partial y_{n+1}^{(i)}} & -\beta_1 - \alpha_1 h \frac{\partial f_{n+2}^{(i)}}{\partial y_{n+2}^{(i)}} & -\gamma_1 - \alpha_1 h \frac{\partial f_{n+3}^{(i)}}{\partial y_{n+3}^{(i)}} \\
    -\beta_2 - \alpha_2 h \frac{\partial f_{n+2}^{(i)}}{\partial y_{n+1}^{(i)}} & 1 - \alpha_2 h \frac{\partial f_{n+2}^{(i)}}{\partial y_{n+2}^{(i)}} & \gamma_2 - \alpha_2 h \frac{\partial f_{n+3}^{(i)}}{\partial y_{n+3}^{(i)}} \\
    -\beta_3 - \alpha_3 h \frac{\partial f_{n+3}^{(i)}}{\partial y_{n+1}^{(i)}} & -\gamma_3 - \alpha_3 h \frac{\partial f_{n+3}^{(i)}}{\partial y_{n+2}^{(i)}} & 1 - \alpha_3 h \frac{\partial f_{n+3}^{(i)}}{\partial y_{n+3}^{(i)}}
\end{bmatrix}.
\]  

(26)

Therefore, the values of \( e_{n+j}^{(i+1)} \) \( j = 1, 2, 3 \) can be approximated and the solutions \( y_{n+j}^{(i+1)} \) \( j = 1, 2, 3 \) are computed from
\[ y_{n+j}^{(i+1)} = y_{n+j}^{(i)} + e_{n+j}^{(i+1)}, \quad j = 1, 2, 3, \]

when \( r = 1, 2, \) and \( \frac{1000}{1196} \).

**Choosing the step size**

Choosing the step size is an important factor in the reduction of the number of iterations. The step size selection falls into three strategies. Using a prescribed tolerance value (TOL), an initial step size is determined. A test is conducted to compare the local truncation error (LTE) with TOL, where

\[ LTE = |y_{n+3}^{(k)} - y_{n+3}^{(k-1)}|, \quad k = 6. \]

If the LTE < TOL, the step is considered as successful (IST). At this step, the previous step size is maintained (corresponding to using \( r = 1 \)) and the following test will be conducted:

\[ h_{\text{new}} = c \times h_{\text{old}} \times \left( \frac{TOL}{LTE} \right)^{\frac{1}{k}}, \]

where \( c \) is the safety factor, \( k \) is the order of the method and is equal to 6. \( h_{\text{new}} \) and \( h_{\text{old}} \) are the step size for the current and previous blocks, respectively. Here \( c \) is 0.5. If \( h_{\text{new}} > (1.196) \times h_{\text{old}} \), then \( h_{\text{new}} = (1.196) \times h_{\text{old}} \). This corresponds to using the formula \( r = \frac{1000}{1196} \). On the other hand, if LTE > TOL, the step size is halved and we regard this step as a failed step (ISFT) (corresponding to the formula when \( r = 2 \)).

**6. Numerical Results**

In this section, the numerical results of the 3-point block BDF method of order 6 on a set of stiff problems for tolerances \( 10^{-2}, 10^{-4}, \) and \( 10^{-6} \) are tabulated and compared with MATLAB’s stiff numerical solvers for ODEs as ode15s and ode23s [15]. The maximum global error and the total number of steps for each problem are given. The test problems and their solutions are listed as...
Problem 1 ([18]).
\[ y' = -20y + 24, \quad y(0) = 0, \quad 0 \leq x \leq 10. \]

Exact solution
\[ y(x) = \frac{6}{5} - \frac{6}{5} e^{-20x}. \]

Problem 2 ([6, 8]).
\[ y' = -100(y - x) + 1, \quad y(0) = 1, \quad 0 \leq x \leq 10. \]

Exact solution
\[ y(x) = e^{-100x} + x. \]

Eigenvalue: \( \lambda = -100. \)

Problem 3 ([8]).
\[
\begin{align*}
  y'_1 &= -1002y_1 + 1000y_2^0, \quad y_1(0) = 1, \quad 0 \leq x \leq 20, \\
  y'_2 &= y_1 - y_2(1 + y_2), \quad y_2(0) = 0.
\end{align*}
\]

Exact solution
\[
\begin{align*}
  y_1 &= e^{-2x}, \\
  y_2 &= e^{-x}.
\end{align*}
\]

Eigenvalues: \( \lambda_1 = -2 \) and \( \lambda_2 = -1. \)

Problem 4 ([18]).
\[
\begin{align*}
  y'_1 &= 998y_1 + 1998y_2, \quad y_1(0) = 1, \quad 0 \leq x \leq 10, \\
  y'_2 &= -999y_1 - 1999y_2, \quad y_2(0) = 2.
\end{align*}
\]

Exact solution
\[
\begin{align*}
  y_1 &= 2e^{-x} - e^{-1000x}, \\
  y_2 &= e^{-x} + e^{-1000x}.
\end{align*}
\]
Eigenvalues: $\lambda_1 = -1$ and $\lambda_2 = -1000$.

The notations used in the tables, are listed below:

- **3BBDF**: 3-point variable step block BDF method.
- **TNS**: the total number of steps.
- **TOL**: tolerance value.
- **MAXE**: maximum global error.

### Table 2. Comparison for Problem 1

<table>
<thead>
<tr>
<th>TOL</th>
<th>Method</th>
<th>TNS</th>
<th>MAXE</th>
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</thead>
<tbody>
<tr>
<td>$10^{-2}$</td>
<td>ode15s</td>
<td>29</td>
<td>8.700e-3</td>
</tr>
<tr>
<td></td>
<td>ode23s</td>
<td>19</td>
<td>4.800e-3</td>
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<tr>
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<td>3BBDF</td>
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<tr>
<td>$10^{-4}$</td>
<td>ode15s</td>
<td>61</td>
<td>1.7046e-4</td>
</tr>
<tr>
<td></td>
<td>ode23s</td>
<td>43</td>
<td>2.7400e-4</td>
</tr>
<tr>
<td></td>
<td>3BBDF</td>
<td>123</td>
<td>2.1979e-8</td>
</tr>
<tr>
<td>$10^{-6}$</td>
<td>ode15s</td>
<td>96</td>
<td>2.7175e-6</td>
</tr>
<tr>
<td></td>
<td>ode23s</td>
<td>148</td>
<td>1.3309e-5</td>
</tr>
<tr>
<td></td>
<td>3BBDF</td>
<td>150</td>
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</tr>
</tbody>
</table>

### Table 3. Comparison for Problem 2

<table>
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<th>Method</th>
<th>TNS</th>
<th>MAXE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-2}$</td>
<td>ode15s</td>
<td>28</td>
<td>8.4000e-3</td>
</tr>
<tr>
<td></td>
<td>ode23s</td>
<td>19</td>
<td>4.5000e-3</td>
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<td>3BBDF</td>
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<td>$10^{-4}$</td>
<td>ode15s</td>
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<td>1.6621e-4</td>
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<tr>
<td></td>
<td>ode23s</td>
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<tr>
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<td>ode15s</td>
<td>100</td>
<td>2.7506e-6</td>
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<tr>
<td></td>
<td>ode23s</td>
<td>143</td>
<td>1.2514e-5</td>
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<td>158</td>
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</tbody>
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Table 4. Comparison for Problem 3

<table>
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<th>TOL</th>
<th>Method</th>
<th>TNS</th>
<th>MAXE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-2}$</td>
<td>ode15s</td>
<td>29</td>
<td>5.2000e-3</td>
</tr>
<tr>
<td></td>
<td>ode23s</td>
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<td>1.1000e-3</td>
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<td>1.7933e-7</td>
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<td>ode15s</td>
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<td>8.5506e-5</td>
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<td>ode23s</td>
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<td>4.9733e-9</td>
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<tr>
<td>$10^{-6}$</td>
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<td>1.0790e-6</td>
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<td></td>
<td>ode23s</td>
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<td></td>
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</tbody>
</table>

Table 5. Comparison for Problem 4

<table>
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<th>TOL</th>
<th>Method</th>
<th>TNS</th>
<th>MAXE</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-2}$</td>
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<td>1.7600e-2</td>
</tr>
<tr>
<td></td>
<td>ode23s</td>
<td>23</td>
<td>7.3000e-3</td>
</tr>
<tr>
<td></td>
<td>3BBDF</td>
<td>118</td>
<td>1.0267e-4</td>
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<tr>
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<td>ode15s</td>
<td>90</td>
<td>1.8559e-4</td>
</tr>
<tr>
<td></td>
<td>ode23s</td>
<td>68</td>
<td>3.6837e-4</td>
</tr>
<tr>
<td></td>
<td>3BBDF</td>
<td>144</td>
<td>1.0882e-6</td>
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<tr>
<td>$10^{-6}$</td>
<td>ode15s</td>
<td>162</td>
<td>3.9569e-6</td>
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<tr>
<td></td>
<td>ode23s</td>
<td>288</td>
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<tr>
<td></td>
<td>3BBDF</td>
<td>171</td>
<td>1.1006e-8</td>
</tr>
</tbody>
</table>

From Tables 2-5, it can be observed that the maximum global error for each given tolerance has decreased in the 3-point block BDF method which shows that the method converges faster for all the problems tested in comparison with ode15s and ode23s.
7. Conclusion

A formulation of a block BDF that computes three points concurrently for the solution of stiff ODEs is considered in this paper. The method is analyzed and is found to be $A$-stable when $r = 2$ and stiffly stable when $r = 1$ and $r = \frac{1000}{1196}$. The results obtained indicate that the code developed is a better solver for stiff problems in reducing the error in comparison with stiff MATLAB’s solvers. In fact, the method outperformed the ode15s and ode23s in terms of accuracy.

Acknowledgement

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References


