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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

$$y' = f(x, y), \quad y(x_0) = y_0, \quad a \leqslant x \leqslant b. \tag{1}$$

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 cuncurently 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).

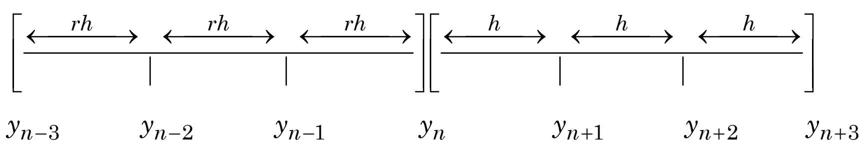

Figure 1. Interpolation points involved in the 3-point variable step BBDF.

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

$$L_{k,j}(x) = \prod_{\substack{i=0 \\ i \neq j}} \frac{x - x_{n+3-i}}{x_{n+3-j} - x_{n+3-i}} \text{ for } j = 0, 1, \ldots, k \ (k = 6),$$

the associated polynomial for (2) can be written as

$$\begin{aligned}
P(x) = \\
& \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+2})}{(x_{n+3} - x_{n-3})(x_{n+3} - x_{n-2})(x_{n+3} - x_{n-1})(x_{n+3} - x_n)(x_{n+3} - x_{n+1})(x_{n+3} - x_{n+2})} y_{n+3} \\
& + \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+3})}{(x_{n+2} - x_{n-3})(x_{n+2} - x_{n-2})(x_{n+2} - x_{n-1})(x_{n+2} - x_n)(x_{n+2} - x_{n+1})(x_{n+2} - x_{n+3})} y_{n+2} \\
& + \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+2})(x - x_{n+3})}{(x_{n+1} - x_{n-3})(x_{n+1} - x_{n-2})(x_{n+1} - x_{n-1})(x_{n+1} - x_n)(x_{n+1} - x_{n+2})(x_{n+1} - x_{n+3})} y_{n+1} \\
& + \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n+1})(x - x_{n+2})(x - x_{n+3})}{(x_n - x_{n-3})(x_n - x_{n-2})(x_n - x_{n-1})(x_n - x_{n+1})(x_n - x_{n+2})(x_n - x_{n+3})} y_n \\
& + \frac{(x - x_{n-3})(x - x_{n-2})(x - x_n)(x - x_{n+1})(x - x_{n+2})(x - x_{n+3})}{(x_{n-1} - x_{n-3})(x_{n-1} - x_{n-2})(x_{n-1} - x_n)(x_{n-1} - x_{n+1})(x_{n-1} - x_{n+2})(x_{n-1} - x_{n+3})} y_{n-1} \\
& + \frac{(x - x_{n-3})(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+2})(x - x_{n+3})}{(x_{n-2} - x_{n-3})(x_{n-2} - x_{n-1})(x_{n-2} - x_n)(x_{n-2} - x_{n+1})(x_{n-2} - x_{n+2})(x_{n-2} - x_{n+3})} y_{n-2} \\
& + \frac{(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+2})(x - x_{n+3})}{(x_{n-3} - x_{n-2})(x_{n-3} - x_{n-1})(x_{n-3} - x_n)(x_{n-3} - x_{n+1})(x_{n-3} - x_{n+2})(x_{n-3} - x_{n+3})} y_{n-3}.
\end{aligned} \tag{3}$$

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

$$\begin{aligned}
p(x) &= p(x_{n+1} + sh) \\
&= \frac{(s + 1 + 3r)(s + 1 + 2r)(s + 1 + r)(s + 1)s(s - 1)}{6(3 + 3r)(3 + 2r)(3 + r)} y_{n+3} \\
&\quad + \frac{(s + 1 + 3r)(s + 1 + 2r)(s + 1 + r)(s + 1)s(s - 2)}{(-2)(2 + 3r)(2 + 2r)(2 + r)} y_{n+2} \\
&\quad + \frac{(s + 1 + 3r)(s + 1 + 2r)(s + 1 + r)(s + 1)(s - 1)(s - 2)}{2(1 + 3r)(1 + 2r)(1 + r)} y_{n+1}
\end{aligned}$$

$$+\frac{(s+1+3r)(s+1+2r)(s+1+r)s(s-1)(s-2)}{(-36)r^3}y_n$$

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

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

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

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

$$hf_{n+1} = \frac{-(6r^2+5r+1)}{18(r+3)(2r+3)}y_{n+3}+\frac{6r^2+5r+1}{2(r+2)(3r+2)}y_{n+2}$$

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

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

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

$$hf_{n+2} = \frac{2(3r^2+8r+4)}{9(r+3)(2r+3)}y_{n+3}+\frac{3r^3+22r^2+36r+16}{2(r+1)(r+2)(3r+2)}y_{n+2}$$

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

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

$$+\frac{(-2)(r+2)}{9r^3(3r+1)(3r+2)}y_{n-3}; \tag{6}$$

$$hf_{n+3} = \frac{22r^3 + 143r^2 + 270r + 153}{6(r+1)(r+3)(2r+3)} y_{n+3} + \frac{(-9)(2r^2 + 9r + 9)}{2(r+2)(3r+2)} y_{n+2}$$

$$+ \frac{9(2r^2 + 9r + 9)}{2(2r+1)(3r+1)} y_{n+1} + \frac{-(2r^3 + 11r^2 + 18r + 9)}{6r^3} y_n$$

$$+ \frac{9(2r+3)}{r^3(r+2)(r+3)} y_{n-1} + \frac{(-9)(r+3)}{r^3(2r+1)(2r+3)} y_{n-2}$$

$$+ \frac{2r^2 + 9r + 9}{3r^3(r+1)(3r+1)(3r+2)} y_{n-3}. \tag{7}$$

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 $r = 1$,

$$y_{n+1} = -\frac{1}{35} y_{n-3} + \frac{8}{35} y_{n-2} - \frac{6}{7} y_{n-1} + \frac{16}{7} y_n - \frac{24}{35} y_{n+2} + \frac{2}{35} y_{n+3} + \frac{12}{7} hf_{n+1},$$

$$y_{n+2} = \frac{2}{77} y_{n-3} - \frac{15}{77} y_{n-2} + \frac{50}{77} y_{n-1} - \frac{100}{77} y_n + \frac{150}{77} y_{n+1} - \frac{10}{77} y_{n+3} + \frac{60}{77} hf_{n+2},$$

$$y_{n+3} = -\frac{10}{147} y_{n-3} + \frac{24}{49} y_{n-2} - \frac{75}{49} y_{n-1} + \frac{400}{147} y_n - \frac{150}{49} y_{n+1} + \frac{120}{49} y_{n+2} + \frac{20}{49} hf_{n+3}. \tag{8}$$

For $r = 2$,

$$y_{n+1} = -\frac{25}{3552} y_{n-3} + \frac{21}{296} y_{n-2} - \frac{245}{592} y_{n-1} + \frac{1225}{296} y_n - \frac{3675}{1184} y_{n+2} + \frac{35}{111} y_{n+3}$$

$$+ \frac{210}{37} hf_{n+1},$$

$$y_{n+2} = \frac{1}{325} y_{n-3} - \frac{16}{875} y_{n-2} + \frac{12}{125} y_{n-1} - \frac{16}{25} y_n + \frac{1536}{875} y_{n+1} - \frac{512}{2652} y_{n+3}$$

$$+ \frac{24}{25} hf_{n+2},$$

$$
\begin{aligned}
y_{n+3} = & -\frac{175}{46112} y_{n-3} + \frac{405}{11528} y_{n-2} - \frac{3969}{23056} y_{n-1} + \frac{11025}{11528} y_n - \frac{2835}{1441} y_{n+1} \\
& + \frac{99225}{46112} y_{n+2} + \frac{630}{1441} hf_{n+3}. \qquad (9)
\end{aligned}
$$

For $r = \dfrac{1000}{1196}$,

$$
\begin{aligned}
y_{n+1} = & -\frac{311249130548929261}{6821843556718750000} y_{n-3} + \frac{4828453731348401349}{14139637164296875000} y_{n-2} \\
& - \frac{5614735319756923077601}{4922334619068125000000} y_{n-1} + \frac{23525925341746689}{10121429609375000} y_n \\
& - \frac{385670907241749}{740470187020480} y_{n+2} + \frac{42852323026861}{1037962484956705} y_{n+3} \\
& + \frac{920289798}{647771495} hf_{n+1},
\end{aligned}
$$

$$
\begin{aligned}
y_{n+2} = & \frac{21912216496200784}{432892639115234375} y_{n-3} - \frac{163183509197182087744}{460625417024158203125} y_{n-2} \\
& + \frac{498329846860832181}{473334468126953125} y_{n-1} - \frac{683744261438016}{412671724609375} y_n \\
& + \frac{358685514196992}{177091183950373} y_{n+1} - \frac{39853946021888}{338559105010357} y_{n+3} \\
& + \frac{156891024}{211287923} hf_{n+2},
\end{aligned}
$$

$$
\begin{aligned}
y_{n+3} = & -\frac{20521277884988304247681}{145166330275394093750000} y_{n-3} + \frac{155864674783310403807}{164050399688328125000} y_{n-2} \\
& - \frac{231213758866944231807}{87055531248875000000} y_{n-1} + \frac{773863453129498281}{205319649171875000} y_n \\
& - \frac{38058858350631063}{11013687633475597} y_{n+1} + \frac{38058858350631063}{15020909583805888} y_{n+2} \\
& + \frac{5278170546}{13140457547} hf_{n+3}. \qquad (10)
\end{aligned}
$$

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

$$+\frac{1}{35}y_{n-3} - \frac{8}{35}y_{n-2} + \frac{6}{7}y_{n-1} - \frac{16}{7}y_n + y_{n+1} + \frac{24}{35}y_{n+2} - \frac{2}{35}y_{n+3} = \frac{12}{7}hf_{n+1},$$

$$-\frac{2}{77}y_{n-3} + \frac{15}{77}y_{n-2} - \frac{50}{77}y_{n-1} + \frac{100}{77}y_n - \frac{150}{77}y_{n+1} + y_{n+2} + \frac{10}{77}y_{n+3} = \frac{60}{77}hf_{n+2},$$

$$+\frac{10}{147}y_{n-3} - \frac{24}{49}y_{n-2} + \frac{75}{49}y_{n-1} - \frac{400}{147}y_n + \frac{150}{49}y_{n+1} - \frac{120}{49}y_{n+2} + y_{n+3} = \frac{20}{49}hf_{n+3}. \tag{11}$$

The matrix form of (11) is associated with

$$\begin{bmatrix} 0 & 0 & \frac{1}{35} \\ 0 & 0 & -\frac{2}{77} \\ 0 & 0 & \frac{10}{147} \end{bmatrix}\begin{bmatrix} y_{n-5} \\ y_{n-4} \\ y_{n-3} \end{bmatrix} + \begin{bmatrix} -\frac{8}{35} & \frac{6}{7} & -\frac{16}{7} \\ \frac{15}{77} & -\frac{50}{77} & \frac{100}{77} \\ -\frac{24}{49} & +\frac{75}{49} & -\frac{400}{147} \end{bmatrix}\begin{bmatrix} y_{n-2} \\ y_{n-1} \\ y_n \end{bmatrix}$$

$$+\begin{bmatrix} 1 & \frac{24}{35} & -\frac{2}{35} \\ -\frac{150}{77} & 1 & \frac{10}{77} \\ \frac{150}{49} & -\frac{120}{49} & 1 \end{bmatrix}\begin{bmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \end{bmatrix} = \begin{bmatrix} \frac{12}{7} & 0 & 0 \\ 0 & \frac{60}{77} & 0 \\ 0 & 0 & \frac{20}{49} \end{bmatrix}\begin{bmatrix} f_{n+1} \\ f_{n+2} \\ f_{n+3} \end{bmatrix}. \tag{12}$$

Let

$$\alpha_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \ \alpha_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \ \alpha_2 = \begin{bmatrix} \frac{1}{35} \\ -\frac{2}{77} \\ \frac{10}{147} \end{bmatrix}, \ \alpha_3 = \begin{bmatrix} -\frac{8}{35} \\ \frac{15}{77} \\ -\frac{24}{49} \end{bmatrix}, \ \alpha_4 = \begin{bmatrix} \frac{6}{7} \\ -\frac{50}{77} \\ \frac{75}{49} \end{bmatrix},$$

$$\alpha_5 = \begin{bmatrix} -\frac{16}{7} \\ \frac{100}{77} \\ -\frac{400}{147} \end{bmatrix}, \alpha_6 = \begin{bmatrix} 1 \\ -\frac{150}{77} \\ \frac{150}{49} \end{bmatrix}, \alpha_7 = \begin{bmatrix} \frac{24}{35} \\ 1 \\ -\frac{120}{49} \end{bmatrix}, \alpha_8 = \begin{bmatrix} -\frac{2}{35} \\ \frac{10}{77} \\ 1 \end{bmatrix},$$

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

The linear difference operator L is defined by

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

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

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

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,

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

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

$$c_2 = \sum_{j=0}^{8} \frac{(j^2\alpha_j)}{2!} - \sum_{j=0}^{8} (j\beta_j) = 0,$$

$$\vdots$$

$$c_5 = \sum_{j=0}^{8} \frac{(j^5 \alpha_j)}{5!} - \sum_{j=0}^{8} \frac{(j^4 \beta_j)}{4!} = 0,$$

$$c_6 = \sum_{j=0}^{8} \frac{(j^6 \alpha_j)}{6!} - \sum_{j=0}^{8} \frac{(j^5 \beta_j)}{5!} = 0,$$

$$c_7 = \sum_{j=0}^{8} \frac{(j^7 \alpha_j)}{7!} - \sum_{j=0}^{8} \frac{(j^6 \beta_j)}{6!} = \begin{bmatrix} -\frac{4}{245} \\ \frac{10}{539} \\ -\frac{20}{343} \end{bmatrix} \neq \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

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 $|r_s| < 1$, $s = 1, 2, \ldots, k$.

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

$$y' = \lambda y \ (\lambda < 0, \ \lambda \text{ complex}),$$

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

$$AY_m = BY_{m-1} + CY_{m-2}, \tag{15}$$

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,

$$\begin{aligned}\text{(i) } R(t, \hat{h}) = & -\frac{1}{79233}t^2 + \frac{40}{2401}t^3 + \frac{232}{26411}t^3\hat{h} + \frac{1852}{2401}t^4 + \frac{20640}{26411}t^4\hat{h} \\ & + \frac{2400}{26411}t^4\hat{h}^2 - \frac{286568}{79233}t^5 - \frac{72216}{26411}t^5\hat{h} - \frac{109920}{26411}t^5\hat{h}^2 \\ & + \frac{10673}{3773}t^6 - \frac{109036}{26411}t^6\hat{h} + \frac{8880}{3773}t^6\hat{h}^2 - \frac{14400}{26411}t^6\hat{h}^3 \\ = & \ 0; \end{aligned} \tag{16}$$

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

$$\begin{aligned}\text{(iii) } R(t, \hat{h}) = & -\frac{1364796263626722791834314124577555 4499}{21954171420057676926833094421386718750 0000}t^2 \\ & + \frac{9490509363205766214390132478878357434499}{21954171420057676926833094421386718750 0000}t^3 \\ & + \frac{55697423430706601154152884699292 7579}{2310965412637650202824536254882 8125000}t^3\hat{h} \\ & + \frac{2480401684845426196050665771142935 1187}{21954171420057676926833094421386718750}t^4 \\ & + \frac{115028677210765616692778596732358021703}{878166856802307077073323776855468 75000}t^4\hat{h} \\ & + \frac{2801303270263832633162046362322}{1878431779256271822616735351 5625}t^4\hat{h}^2 \\ & - \frac{51549616346796725721498180765423 27}{1405066970883691323317318042968750}t^5 \\ & - \frac{1297010472298974226423732248769653}{7025334854418456616586590214843 75}t^5\hat{h} \end{aligned}$$

$$
\begin{aligned}
&- \frac{16434958044578911094654822596929444}{3512667427209228308293295107421875} t^5 \hat{h}^2 \\
&+ \frac{9226662658933489037771816}{3696784630485354355285 03} t^6 \\
&- \frac{126553502859219440595 2407968}{359697144546224978769233419} t^6 \hat{h} \\
&+ \frac{355603853882525421970 2996}{184839231524267717764 2515} t^6 \hat{h}^2 \\
&- \frac{40753462903043087608 94016}{96175707097921117317 97685} t^6 \hat{h}^3 \\
&= 0. \qquad (18)
\end{aligned}
$$

For zero stability, we set $\hat{h} = 0$ in (16), (17), and (18) to obtain the first characteristic polynomial as

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

$$
\begin{aligned}
\text{(ii)} \ &\frac{1996376}{266585} t^6 - \frac{157887}{20350} t^5 + \frac{359023}{1332925} t^4 + \frac{22257}{42653600} t^3 \\
&- \frac{1}{42653600} t^2 = 0; \qquad (20)
\end{aligned}
$$

$$
\begin{aligned}
\text{(iii)} \ &+ \frac{9226662658933489037771816}{369678463048535435528503} t^6 \\
&- \frac{5154961634679672572149818076542327}{1405066970883691323317318042968750} t^5 \\
&+ \frac{248040168484542619605066577114293511 87}{21954171420057676926833094421386718750} t^4 \\
&+ \frac{949050936320576621439013247887835743 4499}{21954171420057676926833094421386718750 0000} t^3 \\
&- \frac{136479626362672279183431412457755544 99}{21954171420057676926833094421386718750 0000} t^2 \\
&= 0. \qquad (21)
\end{aligned}
$$

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.

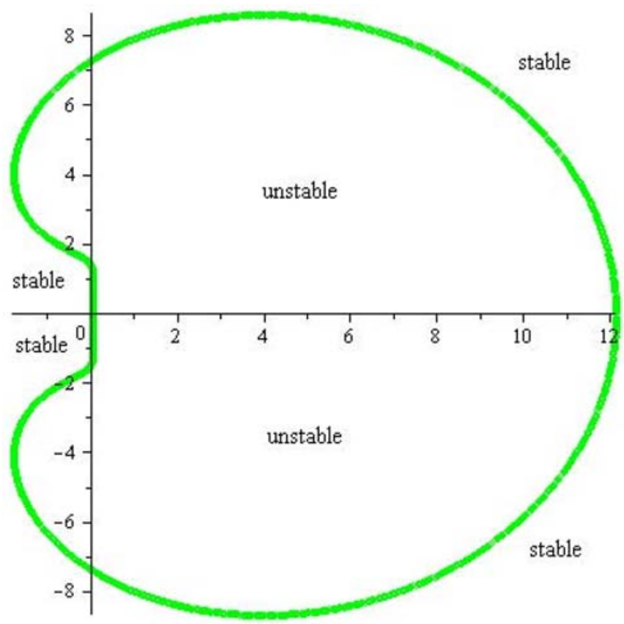

Figure 2. Stability region when $r = 1$.

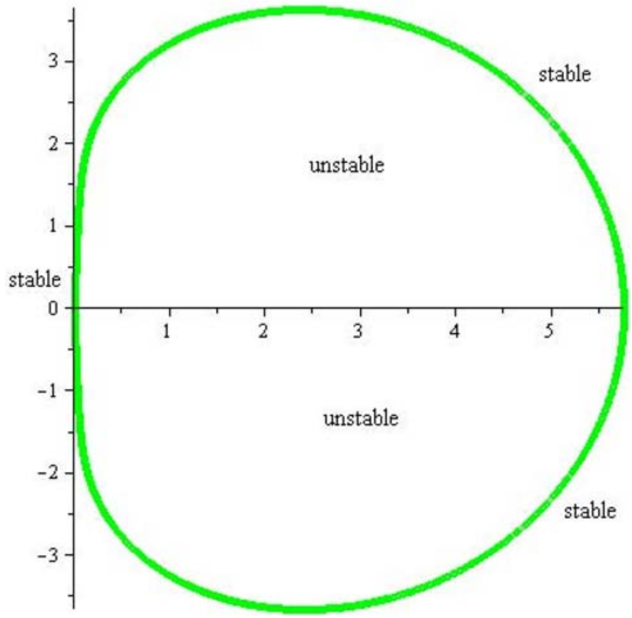

Figure 3. Stability region when $r = 2$.

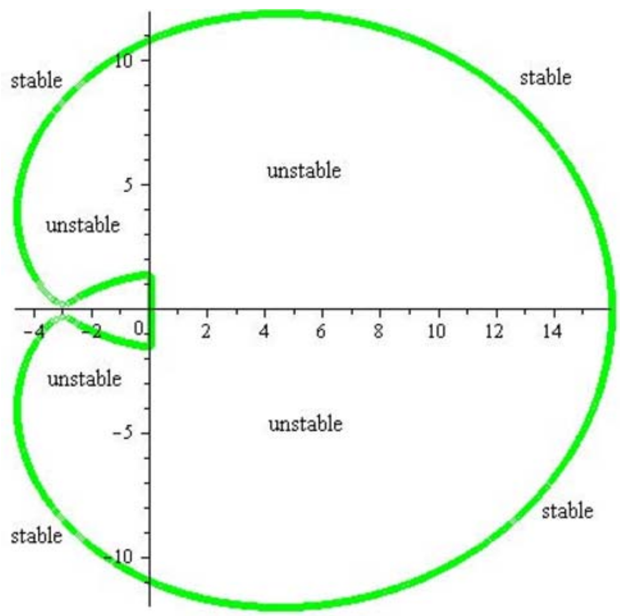

Figure 4. Stability region when $r = \frac{1000}{1196}$.

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

r	$\frac{1}{r}$	Status of the method
$\frac{1}{2}$	2	not zero stable
$r = \frac{10}{19}$	1.9	not zero stable
$r = \frac{5}{8}$	1.6	not zero stable
$r = \frac{2}{3}$	1.5	zero stable not absolutely stable
$r = \frac{5}{7}$	1.4	zero stable not absolutely stable
$r = \frac{10}{13}$	1.3	zero stable not absolutely stable
$r = \frac{5}{6}$	1.2	zero stable not absolutely stable
$r = \frac{1000}{1198}$	1.1198	zero stable not absolutely stable
$r = \frac{1000}{1197}$	1.1197	zero stable not absolutely stable
$r = \frac{1000}{1196}$	1.1196	zero stable and absolutely stable

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 $r = \frac{2}{3}, \frac{5}{7}, \frac{10}{13}, \frac{5}{6}, \frac{1000}{1198},$ 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 $r = \frac{1000}{1198}, \frac{5}{6}, \frac{10}{13}, \frac{5}{7},$ 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 $r = \frac{1000}{1197}, \frac{1000}{1198}, \frac{5}{6}, \frac{10}{13}, \frac{5}{7},$ and $\frac{2}{3}$.

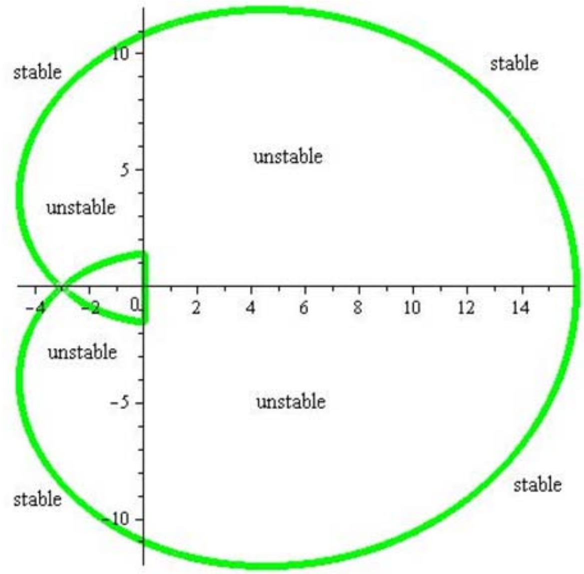

Figure 5. Stability region when $r = \dfrac{1000}{1197}$.

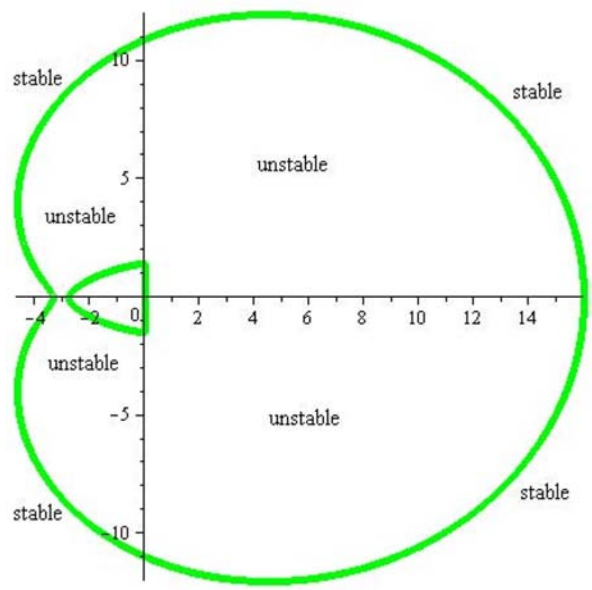

Figure 6. Stability region when $r = \dfrac{1000}{1198}$.

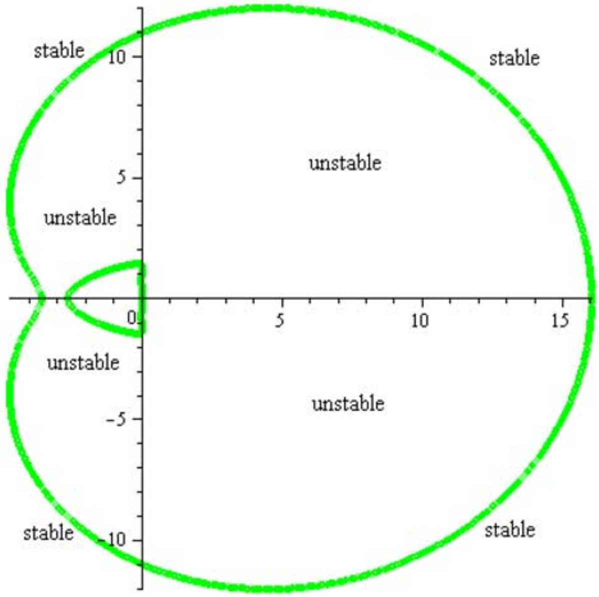

Figure 7. Stability region when $r = \frac{5}{6}$.

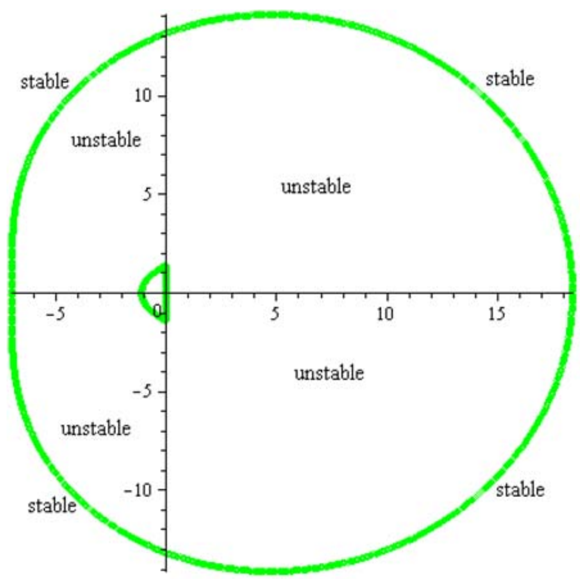

Figure 8. Stability region when $r = \frac{10}{13}$.

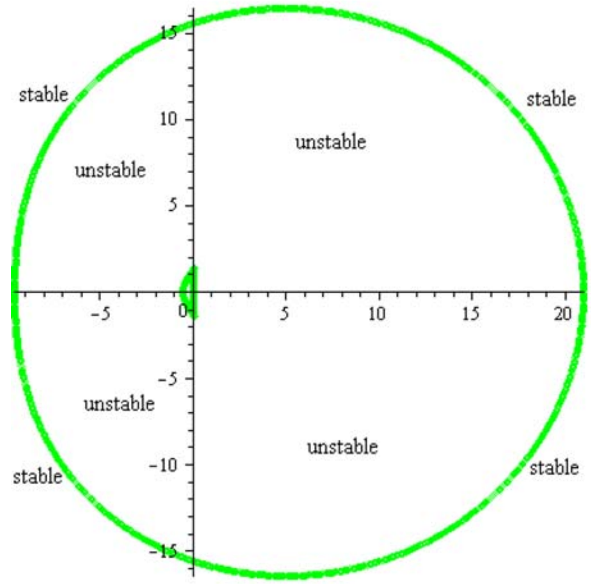

Figure 9. Stability region when $r = \frac{5}{7}$.

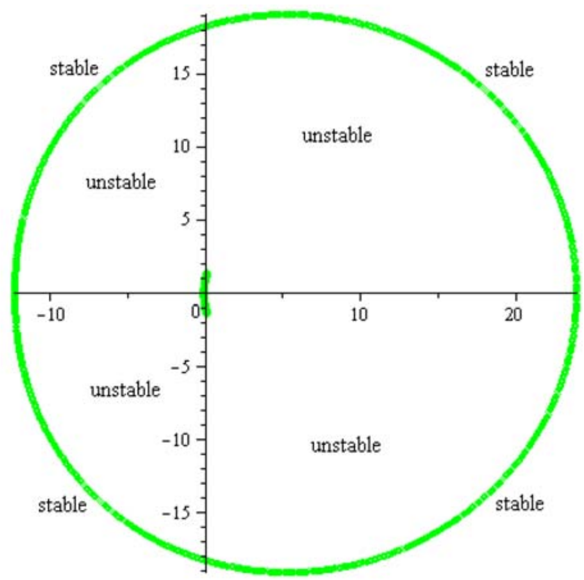

Figure 10. Stability region when $r = \frac{2}{3}$.

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 $(i)^{\text{th}}$ iteration as

$$\text{error}^{(i)} = |y^{(i)}_{\text{exact}} - y^{(i)}_{\text{approximate}}|,$$

and the maximum error is given by

$$MAXE = \max_{1 \leqslant i \leqslant TNS}(\text{error}^{(i)}).$$

The abbreviation TNS gives the total number of steps.

Let $y^{(i+1)}_{n+j} j = 1, 2, 3$ denote the $(i+1)^{\text{th}}$ iterative values of y_{n+j}, define

$$e^{(i+1)}_{n+j} = y^{(i+1)}_{n+j} - y^{(i)}_{n+j}, \quad j = 1, 2, 3.$$

The 3-point block BDF method can be written as

$$\begin{aligned} y_{n+1} &= \alpha_1 hf_{n+1} + \beta_1 y_{n+2} + \gamma_1 y_{n+3} + \eta_1, \\ y_{n+2} &= \alpha_2 hf_{n+2} + \beta_2 y_{n+1} + \gamma_2 y_{n+3} + \eta_2, \\ y_{n+3} &= \alpha_3 hf_{n+3} + \beta_3 y_{n+1} + \gamma_3 y_{n+2} + \eta_3, \end{aligned} \tag{22}$$

where α_i, β_i, and γ_i, $i = 1, 2, 3$ represent the coefficients when $r = 1, 2,$ and $\frac{1000}{1196}$, respectively. η_1, η_2 and η_3 represent the back values. Let

$$\begin{aligned} F_1 &= y_{n+1} - \beta_1 y_{n+2} - \gamma_1 y_{n+3} - \alpha_1 hf_{n+1} - \eta_1, \\ F_2 &= -\beta_2 y_{n+1} + y_{n+2} - \gamma_2 y_{n+3} - \alpha_2 hf_{n+2} - \eta_2, \\ F_3 &= -\beta_3 y_{n+1} - \gamma_3 y_{n+2} + y_{n+3} - \alpha_3 hf_{n+3} - \eta_3. \end{aligned} \tag{23}$$

Newton's iteration is defined as

$$y^{(i+1)}_{n+j} = y^{(i)}_{n+j} - \left[\frac{\partial F^{(i)}_j}{\partial y^{(i)}_{n+j}} \right]^{-1} F^{(i)}_j, \quad j = 1, 2, 3.$$

Hence, Newton's iteration can be defined in the form

$$\begin{bmatrix} y_{n+1}^{(i+1)} \\ y_{n+2}^{(i+1)} \\ y_{n+3}^{(i+1)} \end{bmatrix} = \begin{bmatrix} y_{n+1}^{(i)} \\ y_{n+2}^{(i)} \\ y_{n+3}^{(i)} \end{bmatrix} - \begin{bmatrix} \frac{\partial F_1^{(i)}}{\partial y_{n+1}^{(i)}} & \frac{\partial F_1^{(i)}}{\partial y_{n+2}^{(i)}} & \frac{\partial F_1^{(i)}}{\partial y_{n+3}^{(i)}} \\ \frac{\partial F_2^{(i)}}{\partial y_{n+1}^{(i)}} & \frac{\partial F_2^{(i)}}{\partial y_{n+2}^{(i)}} & \frac{\partial F_2^{(i)}}{\partial y_{n+3}^{(i)}} \\ \frac{\partial F_3^{(i)}}{\partial y_{n+1}^{(i)}} & \frac{\partial F_3^{(i)}}{\partial y_{n+2}^{(i)}} & \frac{\partial F_3^{(i)}}{\partial y_{n+3}^{(i)}} \end{bmatrix}^{-1} \cdot \begin{bmatrix} F_1^{(i)} \\ F_2^{(i)} \\ F_3^{(i)} \end{bmatrix}. \tag{24}$$

Equation (24) is equivalent to

$$\underbrace{\begin{bmatrix} \frac{\partial F_1^{(i)}}{\partial y_{n+1}^{(i)}} & \frac{\partial F_1^{(i)}}{\partial y_{n+2}^{(i)}} & \frac{\partial F_1^{(i)}}{\partial y_{n+3}^{(i)}} \\ \frac{\partial F_2^{(i)}}{\partial y_{n+1}^{(i)}} & \frac{\partial F_2^{(i)}}{\partial y_{n+2}^{(i)}} & \frac{\partial F_2^{(i)}}{\partial y_{n+3}^{(i)}} \\ \frac{\partial F_3^{(i)}}{\partial y_{n+1}^{(i)}} & \frac{\partial F_3^{(i)}}{\partial y_{n+2}^{(i)}} & \frac{\partial F_3^{(i)}}{\partial y_{n+3}^{(i)}} \end{bmatrix}}_{\text{Jacobian matrix}} \cdot \begin{bmatrix} e_{n+1}^{(i+1)} \\ e_{n+2}^{(i+1)} \\ e_{n+3}^{(i+1)} \end{bmatrix} = - \begin{bmatrix} F_1^{(i)} \\ F_2^{(i)} \\ F_3^{(i)} \end{bmatrix}. \tag{25}$$

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

$$J = \begin{bmatrix} 1 - \alpha_1 h \frac{\partial f_{n+1}^{(i)}}{\partial y_{n+1}^{(i)}} & -\beta_1 - \alpha_1 h \frac{\partial f_{n+1}^{(i)}}{\partial y_{n+2}^{(i)}} & -\gamma_1 - \alpha_1 h \frac{\partial f_{n+1}^{(i)}}{\partial y_{n+3}^{(i)}} \\ -\beta_2 - \alpha_2 h \frac{\partial f_{n+2}^{(i)}}{\partial y_{n+1}^{(i)}} & 1 - \alpha_2 h \frac{\partial f_{n+2}^{(i)}}{\partial y_{n+2}^{(i)}} & \gamma_2 - \alpha_2 h \frac{\partial f_{n+2}^{(i)}}{\partial y_{n+3}^{(i)}} \\ -\beta_3 - \alpha_3 h \frac{\partial f_{n+3}^{(i)}}{\partial y_{n+1}^{(i)}} & -\gamma_3 - \alpha_3 h \frac{\partial f_{n+3}^{(i)}}{\partial y_{n+2}^{(i)}} & 1 - \alpha_3 h \frac{\partial f_{n+3}^{(i)}}{\partial y_{n+3}^{(i)}} \end{bmatrix}. \tag{26}$$

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

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

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_{new} and h_{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]).

$$y' = -20y + 24, \qquad y(0) = 0, \qquad 0 \leqslant x \leqslant 10.$$

Exact solution

$$y(x) = \frac{6}{5} - \frac{6}{5}e^{-20x}.$$

Problem 2 ([6, 8]).

$$y' = -100(y - x) + 1, \qquad y(0) = 1, \qquad 0 \leqslant x \leqslant 10.$$

Exact solution

$$y(x) = e^{-100x} + x.$$

Eigenvalue: $\lambda = -100$.

Problem 3 ([8]).

$$y_1' = -1002y_1 + 1000y_2^2, \qquad y_1(0) = 1, \qquad 0 \leqslant x \leqslant 20,$$

$$y_2' = y_1 - y_2(1 + y_2), \qquad y_2(0) = 0.$$

Exact solution

$$y_1 = e^{-2x},$$

$$y_2 = e^{-x}.$$

Eigenvalues: $\lambda_1 = -2$ and $\lambda_2 = -1$.

Problem 4 ([18]).

$$y_1' = 998y_1 + 1998y_2, \qquad y_1(0) = 1, \qquad 0 \leqslant x \leqslant 10,$$

$$y_2' = -999y_1 - 1999y_2, \qquad y_2(0) = 2.$$

Exact solution

$$y_1 = 2e^{-x} - e^{-1000x},$$

$$y_2 = -e^{-x} + e^{-1000x}.$$

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 309.

Table 2. Comparison for Problem 1

TOL	Method	TNS	MAXE
10^{-2}	ode15s	29	8.700e-3
	ode23s	19	4.800e-3
	3BBDF	97	2.1678e-6
10^{-4}	ode15s	61	1.7046e-4
	ode23s	43	2.7400e-4
	3BBDF	123	2.1979e-8
10^{-6}	ode15s	96	2.7175e-6
	ode23s	148	1.3309e-5
	3BBDF	150	1.1389e-10

Table 3. Comparison for Problem 2

TOL	Method	TNS	MAXE
10^{-2}	ode15s	28	8.4000e-3
	ode23s	19	4.5000e-3
	3BBDF	105	1.0775e-5
10^{-4}	ode15s	60	1.6621e-4
	ode23s	42	2.5683e-4
	3BBDF	131	1.1068e-7
10^{-6}	ode15s	100	2.7506e-6
	ode23s	143	1.2514e-5
	3BBDF	158	1.3571e-9

Table 4. Comparison for Problem 3

TOL	Method	TNS	MAXE
10^{-2}	ode15s	29	5.2000e-3
	ode23s	25	1.1000e-3
	3BBDF	92	1.7933e-7
10^{-4}	ode15s	55	8.5506e-5
	ode23s	118	6.9774e-5
	3BBDF	117	4.9733e-9
10^{-6}	ode15s	197	1.0790e-6
	ode23s	773	2.8081e-6
	3BBDF	144	9.6267e-10

Table 5. Comparison for Problem 4

TOL	Method	TNS	MAXE
10^{-2}	ode15s	38	1.760e-2
	ode23s	23	7.3000e-3
	3BBDF	118	1.0267e-4
10^{-4}	ode15s	90	1.8559e-4
	ode23s	68	3.6837e-4
	3BBDF	144	1.0882e-6
10^{-6}	ode15s	162	3.9569e-6
	ode23s	288	1.7039e-5
	3BBDF	171	1.1006e-8

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.

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