

Treatment of Stiff Initial Value Problems using Block Backward Differentiation formula

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Abstract

Some Block Backward Differentiation Formulas (BDFs) capable of generating solutions to Stiff initial value problems are derived using Lagrangian interpolation technique. The region of absolute stability of the BDFs are constructed and the nature so obtained establishes some fact about the choice of BDFs for numerical treatment of stiff Problems. The BDFs derived were implemented on some standard stiff initial value Problems. The results show that the 3-point BDF step size ratio with $r = 2$ has the widest region of absolute stability and highest accuracy.

Keywords: Zero stability, Hybrid, k –step, Block methods, first order initial value problem

1.0 Introduction

The quest for efficient numerical methods for solving stiff initial value problems is on the increase. Although over the years attempts have been made to solve stiff problems by different methods, some of these methods have failed due to the nature of stiff problems in general and also failure to satisfy some stability conditions.

An Initial Value problem is said to be stiff if the absolute stability required leads to a much smaller value of step size h than would otherwise be needed to satisfy the accuracy requirements. Stiffness as described in the literature is known to depend on three main factors: accuracy, length of interval and region of absolute stability of the methods used [1].

The choice of Backward Differentiation Formula (BDF) which is a Linear Multistep Method (LMM) is of great importance since this class of methods has been shown to possess A-stability and $A(\alpha)$ stability characteristics which are known to specially handle stiff problems. The BDFs used for stiff problems dated back to Curtiss and Hirschfelder [2] while the Region of Absolute Stability (RAS) of some BDFs were discussed by Gear [3] for $k = 1, 2, \dots, 6$; where all the regions are infinite and corresponding methods are stiffly stable and $A(\alpha)$ stable.

In many areas of applications of pure and applied Sciences where ordinary differential equations emerge, some of such equations are stiff in nature, the solution of these class of stiff problems often pose some level of difficulties that resulted in fewer success of schemes to handle such problems.

Block Methods were first proposed by Milne [4] who used them to derive integration formula as Predictor-Corrector (P-C) algorithms. Rosser [5] developed Milne's methods in form of implicit methods. Shampine and Watts [6] also contributed to the development of block implicit one-step methods while Chu and Hamilton [7] considered some multi-block schemes. Voss and Abass [8] and Ehigie et al. [9] developed some block schemes but they were implemented as P-C mode of Milne. Some other researchers have also derived some block methods using some

Runge Kutta techniques in terms of embedded formula.

Due to great demand for the solution of real life problems of which many result into stiff problems, we shall at this point derive some block BDFs which are being proposed for the solution of some stiff Problems. The schemes produce numerical solutions to ordinary differential equations given some back values $y_{n-3}, y_{n-2}, y_{n-1}$.

Several authors have used various techniques to derive the Backward Differentiation Formula. These methods include interpolation using Lagrangian interpolation polynomial Okunuga et al. [10] or Newton-divided difference polynomial as basis functions, while some others used the collocation methods as introduced by Onumanyi [11].

In this paper we shall use Lagrangian interpolation formula which defines an approximation polynomial

$P_k(x) \approx y(x)$ as the basis function,

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$$P_k(x) = \sum_{j=a}^b L_{k,j}(x)y(x_{n+1-j}) \tag{1.1}$$

$$L_{k,j}(x) = \prod_{i=a, i \neq j}^b \frac{(x - x_{n+1-i})}{(x_{n+1-i} - x_{n+1-j})}$$

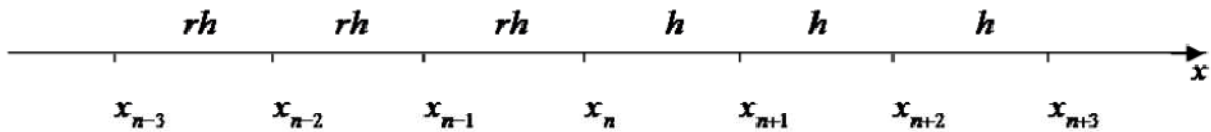
Where x_{n+1-i} , for $i = -m, \dots - 2, -1, 0, 1, 2, \dots, m$ for a m – point block method.

2. Derivation of Block BDFs

Consider the Initial Value Problem,

$$y' = f(x, y), \quad y(x_0) = y_0 \tag{2.1}$$

In order to integrate (2.1), considering that the step size of the computed block is $3h$ and the step size of the previous block is $3rh$ where r is the step size ratio as shown in Figure 1. We consider the values for $r = 1, 2$ and $\frac{1}{2}$ which corresponds to integration with constant step size, halving the step size and doubling the step size respectively. The step size ratios are chosen first, because of stability region and secondly so as to have comparison of our methods with other previous authors who used the same step size ratios.



For a 3-point block method, we set $a = -3$ and $b = 3$ in equation (1.1), so that on interpolation at the point x_{n+1}, x_{n+2}, \dots , the corresponding points y_{n+1}, y_{n+2}, \dots are obtained. The Lagrangian basis function as an approximation to the solution $y(x)$ involving back values $[x_{n-1}, x_{n-2}, x_{n-3}]$ and future values $[x_{n+1}, x_{n+2}, x_{n+3}]$ will be of the form,

$$y(x) = \frac{(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+2})(x - x_{n+3})}{(x_{n-3} - x_{n-2})(x_{n-3} - x_{n-1})(x_{n-3} - x_n)(x_{n-3} - x_{n+1})(x_{n-3} - x_{n+2})(x_{n-3} - x_{n+3})} y_{n-3}$$

$$+ \frac{(x - x_{n-3})(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+2})(x - x_{n+3})}{(x_{n-2} - x_{n-3})(x_{n-2} - x_{n-1})(x_{n-2} - x_n)(x_{n-2} - x_{n+1})(x_{n-2} - x_{n+2})(x_{n-2} - x_{n+3})} y_{n-2}$$

$$+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_n)(x - x_{n+1})(x - x_{n+2})(x - x_{n+3})}{(x_{n-1} - x_{n-3})(x_{n-1} - x_{n-2})(x_{n-1} - x_n)(x_{n-1} - x_{n+1})(x_{n-1} - x_{n+2})(x_{n-1} - x_{n+3})} y_{n-1}$$

$$+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_{n+1})(x - x_{n+2})(x - x_{n+3})}{(x_n - x_{n-3})(x_n - x_{n-2})(x_n - x_{n-1})(x_n - x_{n+1})(x_n - x_{n+2})(x_n - x_{n+3})} y_n \tag{2.2}$$

$$+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+2})(x - x_{n+3})}{(x_{n+1} - x_{n-3})(x_{n+1} - x_{n-2})(x_{n+1} - x_{n-1})(x_{n+1} - x_n)(x_{n+1} - x_{n+2})(x_{n+1} - x_{n+3})} y_{n+1}$$

$$+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+3})}{(x_{n+2} - x_{n-3})(x_{n+2} - x_{n-2})(x_{n+2} - x_{n-1})(x_{n+2} - x_n)(x_{n+2} - x_{n+1})(x_{n+2} - x_{n+3})} y_{n+2}$$

$$+ \frac{(x - x_{n-3})(x - x_{n-2})(x - x_{n-1})(x - x_n)(x - x_{n+1})(x - x_{n+2})}{(x_{n+3} - x_{n-3})(x_{n+3} - x_{n-2})(x_{n+3} - x_{n-1})(x_{n+3} - x_n)(x_{n+3} - x_{n+1})(x_{n+3} - x_{n+2})} y_{n+2}$$

Differentiating (2.2) and evaluating at points x_{n+1}, x_{n+2} and x_{n+3} we obtain a variable block integration formula of the form,

$$\begin{aligned} & \frac{(2r+1)}{9r^3(3r+1)(3r+2)}y_{n-3} - \frac{9(3r+1)}{2r^3(2r+1)(2r+3)}y_{n-2} + \frac{(2r+1)(3r+1)}{r^3(r+1)(r+2)(r+3)}y_{n-1} = hf_{n+1} \\ & - \frac{(r+1)(2r+1)(3r+1)}{18r^3}y_n - \frac{6r^3 - 11r^2 - 18r - 5}{2(3r+1)(2r+1)(r+1)}y_{n+1} + \frac{(2r+1)(3r+1)}{2(3r+2)(r+2)}y_{n+2} \\ & - \frac{(2r+1)(3r+1)}{18(r+3)(2r+3)}y_{n+3} \end{aligned} \tag{2.3}$$

$$\begin{aligned} & \frac{-2(r+2)}{9r^3(3r+1)(3r+2)}y_{n-3} + \frac{(r+2)(3r+2)}{2r^3(2r+1)(r+1)(2r+3)}y_{n-2} + \frac{2(3r+2)}{r^3(r+2)(r+3)}y_{n-1} = hf_{n+2} \\ & + \frac{(3r+2)(r+2)(r+1)}{18r^3}y_n - \frac{3(r+2)(3r+2)}{(3r+1)(2r+1)}y_{n+1} + \frac{(3r+4)(r^2+6r+4)}{2(3r+2)(r+1)(r+2)}y_{n+2} \\ & - \frac{2(r+2)(3r+2)}{9(r+3)(2r+3)}y_{n+3} \end{aligned} \tag{2.4}$$

$$\begin{aligned} & \frac{(2r+3)(r+3)}{3r^3(r+1)(3r+1)(3r+2)}y_{n-3} - \frac{9(r+3)}{2(2r+1)(2r+3)}y_{n-2} + \frac{9(2r+3)}{r^3(r+2)(r+3)}y_{n-1} = hf_{n+3} \\ & - \frac{(2r+3)(r+3)(r+1)}{6r^3}y_n + \frac{9(r+3)(2r+3)}{2(3r+1)(2r+1)}y_{n+1} - \frac{9(r+3)(2r+3)}{2(r+2)(3r+2)}y_{n+2} \\ & - \frac{22r^3 + 143r^2 + 270r + 153}{6(r+1)(2r+3)(r+3)}y_{n+3} \end{aligned} \tag{2.5}$$

To determine the various LMM as a block for the integration of (2.1) and considering the choice of step length, (2.3), (2.4) and (2.5) are simultaneously evaluated at $r = 1, 2,$ and $\frac{1}{2}$ respectively to obtain:

For $r = 1$:

$$\begin{aligned} y_{n+1} &= -\frac{24}{35}y_{n+2} + \frac{2}{35}y_{n+3} + \frac{16}{7}y_n - \frac{6}{7}y_{n-1} + \frac{8}{35}y_{n-2} - \frac{1}{35}y_{n-3} + \frac{12}{7}hf_{n+1} \\ y_{n+2} &= \frac{150}{77}y_{n+1} - \frac{10}{77}y_{n+3} - \frac{100}{77}y_n + \frac{50}{77}y_{n-1} - \frac{15}{77}y_{n-2} + \frac{2}{77}y_{n-3} + \frac{60}{77}hf_{n+2} \end{aligned} \tag{2.6}$$

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

For $r = 2$:

$$\begin{aligned} y_{n+1} &= -\frac{3675}{1184}y_{n+2} + \frac{35}{111}y_{n+3} + \frac{1225}{296}y_n - \frac{245}{592}y_{n-1} + \frac{21}{296}y_{n-2} - \frac{25}{3552}y_{n-3} + \frac{210}{37}hf_{n+1} \\ y_{n+2} &= \frac{1536}{875}y_{n+1} - \frac{512}{2625}y_{n+3} - \frac{16}{25}y_n + \frac{12}{125}y_{n-1} - \frac{16}{875}y_{n-2} + \frac{1}{525}y_{n-3} + \frac{24}{25}hf_{n+2} \end{aligned} \tag{2.7}$$

$$y_{n+3} = -\frac{2835}{1441}y_{n+1} + \frac{99225}{46112}y_{n+2} + \frac{11025}{11528}y_n - \frac{3969}{23056}y_{n-1} + \frac{405}{11528}y_{n-2} - \frac{175}{46112}y_{n-3} + \frac{630}{1441}hf_{n+3}$$

For $r = \frac{1}{2}$

$$\begin{aligned}
 y_{n+1} &= -\frac{15}{56}y_{n+2} + \frac{25}{1344}y_{n+3} + \frac{25}{8}y_n - \frac{20}{7}y_{n-1} + \frac{75}{64}y_{n-2} - \frac{4}{21}y_{n-3} + \frac{15}{16}hf_{n+1} \\
 y_{n+2} &= \frac{735}{319}y_{n+1} - \frac{175}{1914}y_{n+3} - \frac{1225}{319}y_n + \frac{1344}{319}y_{n-1} - \frac{1225}{638}y_{n-2} + \frac{320}{957}y_{n-3} + \frac{210}{319}hf_{n+2} \\
 y_{n+3} &= -\frac{15876}{3265}y_{n+1} + \frac{9072}{3265}y_{n+2} + \frac{7056}{653}y_n - \frac{41472}{3265}y_{n-1} + \frac{3969}{653}y_{n-2} - \frac{3584}{3265}y_{n-3} + \frac{252}{653}hf_{n+3}
 \end{aligned}
 \tag{2.8}$$

3. Implementation of Block BDFs

To Implement the block BDFs, the methods in the block were individually applied to the test problem. From our findings, the first BDF in the block seeking for y_{n+1} was unable to handle the problems as expected. In order for it not to give a wrong prediction which will affect the entire block, the first BDF was entirely ignored for all the block BDFs and the Explicit Euler method was used as a replacement to get a prediction for y_{n+1} and the other methods which seek for y_{n+2} and y_{n+3} are used as the block method. Also, the Newton Iteration techniques will be used in the determination of the values sought for which the Jacobian $\frac{\partial f}{\partial y}$ of the stiff differential equation will be obtained.

4. Stability of Variable Block Integration Formula

From the literature [3, 12], it is known that stability of a LMM determines the manner in which the error is propagated as the numerical computation proceeds. Hence, it would be necessary to investigate the stability properties of the newly developed methods. In this paper, the RAS of the methods are discussed for various step ratios. The boundary locus method will be used to plot the RAS. This is obtained using the first and second characteristic polynomials as,

$$z(\theta) = \frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}$$

where $\rho(e^{i\theta})$ and $\sigma(e^{i\theta})$ are first and second characteristic polynomial of LMM as discussed in Lambert [12]. Resolving (3.1) to real and imaginary parts and evaluating for values of $\theta \in (0, 2\pi)$ gives the region of stability which is plotted on a graph.

However this method was applied to the resulting LMM from the substitution of the first BDF- y_{n+1} in the second BDF- y_{n+2} and thereafter, the first BDF- y_{n+1} and the second BDF were substituted in the last BDF- y_{n+3} in the block. Hence, the RAS of the Various BDFs for $r = 1$, $r = 2$ and $r = \frac{1}{2}$ are given respectively in Figures 2 - 4.

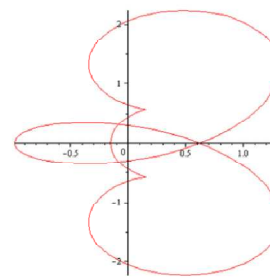
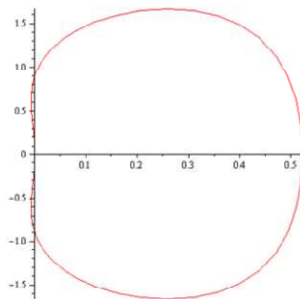
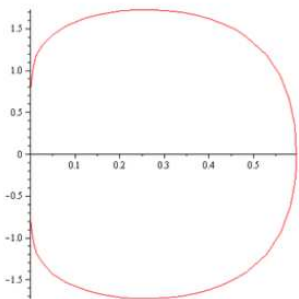


Figure 2: RAS for $r = 1$

Figure 3: RAS for $r = 2$

Figure 4: RAS for $r = \frac{1}{2}$

It is observed that the RAS for $r = 1$ is the widest of all the methods followed by $r = 2$. The nature of the RAS for $r = \frac{1}{2}$ shows that the block BDF at $r = \frac{1}{2}$ is unstable. The Most Interesting property of the BDF for $r = 1$ and $r = 2$ is that the RAS is contained in the left hand half plane and this establishes the A – Stability and $A(\alpha)$ stability properties respectively.

5. Numerical Experiment

In this section, we solve some standard problems with the derived Block BDFs (2.6), (2.7) and (2.8) which shall be denoted as BBDF1, BBDF2 and BBDF3 respectively. The results obtained are compared for various step lengths so as to examine the consistency of the methods on the selected problems, since it has been shown by the RAS that the methods are $A - stable$, $A(\alpha)$ -stable and unstable respectively.

Problem 1

We consider the test problem,

$$y' = \lambda y \tag{5.1}$$

with $\lambda = -1$ and initial values $y(0) = 1$. Solving this problem (5.1) which is known to have an analytical solution:

$y = e^{-x}$ with the BBDF1, BBDF2 and BBDF3 using step length $h = 0.1$ and 0.01 , we obtain the numerical results in terms of the errors in the Table 1:

Table 1: Result of problem 1 for various r values

x	$r = 1$		$r = 2$		$r = \frac{1}{2}$	
	$h = 0.01$	$h = 0.1$	$h = 0.01$	$h = 0.1$		
	BBDF1	BBDF1	BBDF2	BBDF2	BBDF3	BBDF3
0.02	8.25e-05		7.11e-04		6.74e-03	xxx
0.03	4.03e-05		2.86e-04		5.88e-04	
0.1	7.36e-05		8.27e-04		xxx	
0.2	2.37e-04	7.77e-03	1.07e-03	1.23e-02		
0.3	3.35e-04	3.26e-03	1.27e-03	4.18e-03		
0.4	4.37e-04	1.53e-03	1.41e-03	3.49e-03		
0.5	5.07e-04	3.26e-03	1.52e-03	1.43e-04		
0.6	5.60e-04	1.32e-03	1.59e-03	1.75e-03		
0.7	5.99e-04	1.37e-03	1.64e-03	1.66e-03		
0.8	6.25e-04	4.32e-03	1.66e-03	6.90e-04		
0.9	6.41e-04	3.09e-03	1.66e-03	3.08e-03		
1.0	6.48e-04	1.59e-03	1.65e-03	1.98e-03		

xxx- The scheme explodes on evaluation

From the Table 1, it is observed that the BBDF2 gives a result slightly different from the BBDF1 using a step length of 0.1 but on the reduction of the step length to 0.01 the results obtained by the BBDF1 gains slight accuracy while the BBDF2 remains consistent. The BBDF3 gave a favourable numerical solution only in the first block and failed completely thereafter.

Since BBDF3 is unstable as displayed in Figure 4, it is clear that BBDF3 with $r = \frac{1}{2}$ will not be suitable for the integration on stiff problems. Hence we discard the BBDF3.

Problem 2

The Problem 1 is extended to another ordinary differential equation of the form,

$$y' = \lambda(y - x) + 1, \quad y(0) = 1, \quad 0 \leq x \leq 10 \tag{5.2}$$

considered by Ibrahim et al. [13]. This problem is solved for $\lambda = -5$ and $\lambda = -20$. This has an analytical solution given by $y = e^{\lambda x} + x$.

Therefore it is expected that as $\lambda \rightarrow x$, $y \rightarrow x$. Applying the BBDF1, BBDF2 and BBDF3, we present the results in terms of their errors in Tables 2 and 3:

Table 2: Result of Problem 2 with $\lambda = -5$

$\lambda = -5$ x	$r = 1$		$r = 1$	
	$h = 0.01$	$h = 0.1$	$h = 0.01$	$h = 0.1$
	BBDF1	BBDF1	BBDF2	BBDF2
0.02	2.61e-03		4.12e-03	
0.03	9.20e-04		1.55e-03	
0.9	4.35e-04	8.29e-03	1.55e-03	4.19e-04
1	2.96e-04	5.48e-02	1.46e-03	5.39e-04
2	4.55e-06	3.57e-02	1.26e-03	1.04e-04
3	3.27e-06	2.29e-02	1.26e-03	9.64e-04
4	3.34e-06	1.47e-02	1.26e-03	9.63e-04
5	2.86e-06	9.42e-03	1.26e-03	9.63e-04
6	6.20e-06	6.05e-03	1.26e-03	9.63e-04
7	6.20e-06	3.88e-03	1.26e-03	9.63e-04
8	5.27e-06	2.49e-03	1.26e-03	9.63e-04
9	0	1.60e-03	1.26e-03	9.63e-04
10	2.86e-06	1.02e-03	1.26e-03	9.63e-04

Table 3: Result of Problem 2 with $\lambda = -20$

$\lambda = -20$ x	$r = 1$		$r = 1$	
	$h = 0.01$	$h = 0.1$	$h = 0.01$	$h = 0.1$
	BBDF1	BBDF1	BBDF2	BBDF2
0.02	2.90e-02		3.46e-02	
0.03	9.91e-01		1.01e-02	
0.9	2.86e-05	3.32e-01	2.70e-04	1.47e-01
1	1.44e-05	2.74e-01	2.69e-04	1.05e-01
2	1.19e-07	7.68e-02	2.69e-04	1.13e-02
3	0	2.15e-02	2.69e-04	2.31e-04
4	0	6.05e-03	2.69e-04	9.09e-04
5	1.91e-06	1.70e-03	2.68e-04	7.96e-04
6	4.77e-07	4.76e-04	2.68e-04	8.07e-04
7	4.77e-07	1.34e-04	2.68e-04	8.06e-04
8	9.53e-07	3.77e-05	2.68e-04	8.06e-04
9	0	1.44e-05	2.67e-04	8.06e-04
10	0	2.86e-06	2.67e-04	8.06e-04

The results obtained show that the BBDF2 remains consistent for both λ values but BBDF1 has a lesser accuracy than the BBDF2 for $h = 0.1$ but BBDF1 gains better accuracy on the reduction of the step length, while the BBDF2 remains consistent even on reduction of the step length. BBDF3 also failed for both problems of λ due to instability.

Problem 3 (Dahlquist et al. [14])

The stiff problem

$$y' = 100(\sin x - y), \quad y(0) = 0 \tag{5.3}$$

is considered for step length $h = \frac{\pi}{60}$ and $h = \frac{\pi}{30}$ for $x \in [0, 2\pi]$ with analytical solution of

$$y(x) = \frac{\sin x - 0.01 \cos x + 0.01e^{-100x}}{1.0001}.$$

The table of errors is given in Table 4:

Table 3: Result of Problem 2 with $\lambda = -20$

x	$r = 1$		$r = 1$	
	$h = \frac{\pi}{30}$	$h = \frac{\pi}{60}$	$h = \frac{\pi}{30}$	$h = \frac{\pi}{60}$
	BBDF1	BBDF1	BBDF2	BBDF2
$\frac{\pi}{6}$	2.70e-02	1.64e-04	5.37e-02	3.69e-03
$\frac{\pi}{3}$	7.03e-02	5.04e-04	2.07e-02	3.20e-04
$\frac{\pi}{2}$	3.25e-02	1.67e-04	6.29e-04	2.37e-04
$\frac{2\pi}{3}$	1.21e-02	1.15e-06	8.08e-04	1.43e-04
$\frac{5\pi}{6}$	9.56e-03	2.78e-05	7.58e-04	4.69e-04
π	1.27e-02	3.81e-07	1.62e-03	6.70e-04
$\frac{7\pi}{6}$	5.41e-03	4.25e-05	7.49e-04	6.92e-04
$\frac{4\pi}{3}$	3.75e-03	7.64e-05	1.75e-03	5.28e-04
$\frac{3\pi}{2}$	2.77e-02	9.05e-05	2.48e-05	2.22e-04
$\frac{5\pi}{3}$	2.38e-3	8.05e-05	1.27e-04	1.42e-04
$\frac{11\pi}{6}$	6.26e-04	4.88e-05	7.22e-04	4.69e-044
2π	1.08e-3	4.08e-05	1.62e-03	6.70e-04

From Table 4 the method BBDF2 seems to be the more accurate with step length $\frac{\pi}{30}$ but on reduction of the step length to $\frac{\pi}{60}$ the BBDF1 gains better accuracy leaving the BBDF2 consistent as step length reduces.

6. Conclusion

A class of 3 point block BDFs have been derived using the Lagrangian interpolation technique. Their Stability in terms of RAS have been investigated where BBDF1 has shown to be more robust. These methods have also been implemented on some selected stiff ordinary differential equations. It is observed that each method has a special attribute which may determine its choice for the solution of stiff equations.

The BBDF1 is best used when the step length h is very small as this method responds to reduction of step length by gaining more accuracy, while the BBDF2 has shown itself to be more accurate for large step length h and remains consistent even on the reduction of h .

Because the BBDF3 is unstable from the RAS so obtained, it was unable to handle any of the stiff problems considered in this paper.

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