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Implicit Second Derivative Hybrid Backward Differentiation Formula for the Solution of Second Order Ordinary Differential Equations

Y. Skwame,[1] J. Sunday[1], and T. Y. Kyagya[2]
[1]Department of Mathematics, Adamawa State University, Mubi-Nigeria.
[2]Department of Mathematics/Statistics, Federal University, Wukari-Nigeria
Contacts: skwamey@yahoo.com, sunday578@adsu.edu.ng

Abstract

A Hybrid Backward Differentiation Formula (HBDF) of uniform order ten is proposed for the solution of second order stiff Initial Value Problems (IVPs) is studied in this article. The approach adopted for the derivation of backward differentiation formulae involves interpolation and collocation at appropriate selected points. The proposed order ten HBDF for general second order ODEs was found to be consistent, zero-stable and convergent. Numerical evidences show that the method proposed here perform favorable when compared with existing scheme as it yielded better accuracy.

Keywords: Backward differentiation; collocation; HBDF, interpolation; second derivative; stiff IVPs

Introduction

Most of the improvements in the class of Linear Multistep Methods (LMMs) have been based on Backward Differentiation Formula (BDF), because of its special properties. Among the first modifications introduced by different authors was the Extended Backward Differentiation formulas (EBDFs), introduced in 1980 by Cash, in which one-super future point technique was applied. Cash (1981), proposed second derivative EBDFs for the numerical integration of stiff systems. Also, the integration of stiff initial value problems in ODEs using modified extended backward differentiation formula was studied in Cash (1983). The BDFs are implicit linear $k-step$ method with regions of absolute stability large enough to make them relevant to the problem of stiffness. Backward differentiation methods were introduced Curtiss and Hirschfelder (1952), Muhammad and Yahaya (2012), among others. In the early 1950s, as a result of some pioneering work by Curtiss and Hirschfelder (1952), Stuart and Humphries (1996) realized that there was an important class of Ordinary Differential Equations (ODEs), which have become known as stiff equations, which presented a severe challenge to numerical methods that existed at that time. Since then an enormous amount of effort has gone into the analysis of stiff problems and, as a result, many numerical methods have been proposed for their solution. More recently, however, there have been some strong indications that the theory which underpins stiff computation is now quite well understood, and, in particular, the excellent text of Hairer and Wanner, (1996), has helped put this theory on a firm basis. As a result of this, some powerful codes have now been developed and these can solve quite difficult problems in a routine and reliable way.

Interestingly, differential equations arising from the modeling of physical phenomena often do not have exact solutions. Hence, the development of numerical methods to obtain approximate solutions becomes necessary. To that extent, several numerical methods such as finite difference methods, finite element methods and finite volume methods, among others, have been developed based on the nature and type of the differential equation to be solved.

This research focuses on developing a new HBDF for the solution of second order initial value problems of the form,

$$y'' = f(x, y, y'); \quad y(x_0) = a, \quad y'(x_0) = b, \quad a \le x \le b \qquad (1)$$

Block methods for solving problems of the form (1) have initially been proposed by Milne (1953). The Milne's idea was further developed by Rosser (1967) for Runge-Kutta method. Also block BDFs are discussed and developed by many researchers, Jiaxiang and Cameron (1995), Ibrahim, Othman and Suleiman (2007), Akinfenwa, Jator and Yoa (2011, 2013), Ali and Gholamreza (2011), Yahaya and Mohammed (2009, 2010a, 2010b), Fatunla (1991), Raft and Zurmi (2016), Skwame *et. al.* (2017a), Skwame, Kumleng and Bakari (2017b), Tumba, Sabo and Hamadina (2018), among others.

Materials and Methods

We seek an approximation of the form,

$$Y(x)=\sum_{j=0}^{s+r-1}\ell_j x^j \qquad (2)$$

where ℓ_j are unknown coefficients to be determined and $r\ and\ s$ are the numbers of interpolation and collocation points respectively. We then construct our continuous approximation by imposing the following conditions,

$$Y(x)=x_{n+s}^{j},\quad j=0,1,2,\cdots,k-1 \qquad (3)$$

$$Y''(x_{n+k})=f_{n+k} \qquad (4)$$

We note that $y_{n+\mu}$ is the numerical approximation to the analytical solution, $y(x_{n+\mu}),\ f_{n+\mu}=f\left(x_{n+\mu},y_{n+\mu},y'_{n+\mu}\right)$

Equations (3) and (4) lead to a system of (k+1) equations which is solved by Cramer's rule to obtain ℓ_j. Our continuous approximation is constructed by substituting the values of ℓ_j into equation (2). After some manipulation, the continuous method is obtained as,

$$Y(x)=\sum_{j=0}^{k-1}\alpha_j(x)y_{n+j}+h\alpha_\mu(x)y_{n+\mu}+h^2\beta_k(x)f_{n+k} \qquad (5)$$

where $\alpha_j(x),\alpha_\mu(x), and\ \beta_k(x)$ are continuous coefficients to determined. We note that since the general second order ordinary differential equation involves the first derivative, the first derivative formula is given by.

$$Y'(x)=\sum_{j=0}^{k-1}\alpha'_j(x)y_{n+j}+h\alpha'_\mu(x)y_{n+\mu}+h^2\beta'_k(x)f_{n+k} \qquad (6)$$

$$Y'(x)=\delta(x) \qquad (7)$$

$$Y'(a)=\delta_0 \qquad (8)$$

To construction the double-step implicit second derivative backward differentiation formulae with two off-grid points at interpolation and collocation, we use equation (5) to obtain a continuous $2-step$ HBDF with the following specification, $r=1,\ s=10,\ k=2$. We also express $\alpha_j(x),\alpha_\mu(x), and\ \beta_k(x)$ as a functions of t, where $t=\dfrac{x-x_n}{h}$ to obtain the continuous form as follows:

$$\begin{aligned}y(x)=\alpha_0y_n+h\left(\beta_0(x)f_n+\beta_{\frac{1}{2}}(x)f_{n+\frac{1}{2}}+\beta_1(x)f_{n+1}+\beta_{\frac{3}{2}}(x)f_{n+\frac{3}{2}}+\beta_2(x)f_{n+2}\right)+\\ h^2\left(\gamma_0(x)g_n+\gamma_{\frac{1}{2}}(x)g_{n+\frac{1}{2}}+\gamma_1(x)g_{n+1}+\gamma_{\frac{3}{2}}(x)g_{n+\frac{3}{2}}+\gamma_2(x)g_{n+2}\right)\end{aligned} \qquad (9)$$

where

$${}^{j}\alpha_0=0$$

$$\beta_0=th-\frac{1}{136080}t^3h\begin{pmatrix}1833300+6348825t-10818612t^2+10925250t^3-6832800t^4+2601900t^5\\-553280t^6+50400t^7\end{pmatrix}$$

$$\beta_{\frac{1}{2}}=\frac{4}{8505}t^3h\begin{pmatrix}-30240+211680t-532728t^2+690060t^3-512280t^4+220815t^5\\-51520t^6+5040t^7\end{pmatrix}$$

$$\beta_1=\frac{1}{315}t^3h\begin{pmatrix}3780-17955t+34839t^2-34440t^3+18360t^4-5040t^5\\+560t^6\end{pmatrix}$$

$$\beta_{\frac{3}{2}}=\frac{4}{8505}t^3h\begin{pmatrix}-30240+171360t-419832t^2+562380t^3-440280t^4+200655t^5\\-49280t^6+5040t^7\end{pmatrix}$$

$$\beta_2=\frac{1}{136080}t^3h\begin{pmatrix}-200340+1172745t-2993508t^2+4218690t^3-3509280t^4+1714860t^5\\-454720t^6+50400t^7\end{pmatrix}$$

$$\gamma_0=\frac{1}{45360}t^2h^2\begin{pmatrix}22680-126000t+329175t^2-501480t^3+477330t^4-288000t^5\\+107100t^6-22400t^7+2016t^8\end{pmatrix}$$

$$\gamma_{\frac{1}{2}} = \frac{2}{2835} t^3 h^2 \begin{pmatrix} -15120 + 71820t - 148428t^2 + 170520t^3 - 116820t^4 + 47565t^5 \\ -10640t^6 + 1008t^7 \end{pmatrix}$$

$$\gamma_1 = \frac{1}{10} t^3 h^2 \left(15 - 60t + 94t^2 - 64t^3 + 16t^4\right)(t-2)^3$$

$$\gamma_{\frac{3}{2}} = \frac{2}{2835} t^3 h^2 \begin{pmatrix} -5040 + 28980t - 72320t^2 + 99120t^3 - 79740t^4 + 37485t^5 \\ -9520t^6 + 1008t^7 \end{pmatrix}$$

$$\gamma_2 = \frac{1}{45360} t^3 h^2 \begin{pmatrix} -7560 + 44415t - 113904t^2 + 161490t^3 - 135360t^4 + 66780t^5 \\ -17920t^6 + 2016t^7 \end{pmatrix}$$

Evaluating (9) at $x = x_{n+i}$, $i = 0, \frac{1}{2}, 1, \frac{3}{2}, 2$ yields the second derivative HBDF as follows,

$$y_{n+\frac{1}{2}} = y_n + \frac{1}{8709120} h \left(1539551 f_n + 1429936 f_{n+\frac{1}{2}} + 711936 f_{n+1} + 613456 f_{n+\frac{3}{2}} + 59681 f_{n+2}\right)$$
$$+ \frac{1}{2903040} h^2 \left(26051 g_n - 249656 g_{n+\frac{1}{2}} - 183708 g_{n+1} - 49720 g_{n+\frac{3}{2}} - 2237 g_{n+2}\right)$$

$$y_{n+1} = y_n + \frac{1}{136080} h \left(24463 f_n + 52928 f_{n+\frac{1}{2}} + 44928 f_{n+1} + 12608 f_{n+\frac{3}{2}} + 1153 f_{n+2}\right)$$
$$+ \frac{1}{45360} h^2 \left(421 g_n - 3040 g_{n+\frac{1}{2}} - 4536 g_{n+1} - 992 g_{n+\frac{3}{2}} - 43 g_{n+2}\right)$$

$$y_{n+\frac{3}{2}} = y_n + \frac{3}{35840} h \left(2167 f_n + 4912 f_{n+\frac{1}{2}} + 6912 f_{n+1} + 3792 f_{n+\frac{3}{2}} + 137 f_{n+2}\right)$$
$$+ \frac{3}{35840} h^2 \left(113 g_n - 744 g_{n+\frac{1}{2}} - 756 g_{n+1} - 488 g_{n+\frac{3}{2}} - 15 g_{n+2}\right)$$

$$y_{n+2} = y_n + \frac{1}{8505} h \left(1601 f_n + 4096 f_{n+\frac{1}{2}} + 5616 f_{n+1} + 4096 f_{n+\frac{3}{2}} + 1601 f_{n+2}\right)$$
$$+ \frac{1}{2835} h^2 \left(29 g_n - 128 g_{n+\frac{1}{2}} + 128 g_{n+\frac{3}{2}} - 29 g_{n+2}\right)$$

These four set of equations above form the new HBDF for the solution of problems of the form (1).

In this section, the analysis of the basic properties of the newly derived HBDF shall be carried out.

Analysis of Basic Properties of the New HBDF

Order and Error Constants of the HBDF

Definition 1 (Lambert, 1991)

The linear difference operator ℓ associated with a LMM is defined by

$$\ell[y(x), h] = \sum_{j=0}^{k} \left[(a_j y(x+jh) + h\beta_j y'(x+jh) + h^2 \beta_j y''(x+jh)\right] \qquad (10)$$

where $y(x)$ is an arbitrary test function and it is continuously differentiable on $[a, b]$. Expanding $y(x+jh)$ *and* $y'(x+jh)$ as Taylor series about x, and collecting common terms yields

$$\ell[y(x); h] = c_0 y(x) + c_1 h y'(x) + \cdots + c_q h^q y^q(x) + \cdots \qquad (11)$$

where the constant C_q, $q = 0, 1, \cdots$ coefficients are given as follows

$$c_0 = \alpha_0 + \alpha_1 + \quad \cdots + \alpha_k$$
$$c_1 = \alpha_1 + 2\alpha_2 + \quad \cdots + k\alpha_k - (\beta_0 + \beta_1 \cdots \beta_k)$$
$$\vdots$$
$$c_q = \tfrac{1}{q!}(\alpha_1 + 2^q \alpha_2 + \cdots + k^q \alpha_k) - \tfrac{1}{(q-1)!}(\beta_1 + 2^{(q-1)}\beta_2 + \cdots + k^{(q-1)}\beta_k), \quad q = 2,3,\cdots$$

According to Lambert (1973), the method (5) has order p if

$$c_0 = c_1 = \cdots = c_p = c_{p+1} 0 \; and \; c_{p+2} \neq 0$$

c_{p+2} is the error constant, and p is the order of the LMM. Therefore, the new HBDF is of uniform order ten, with error constants given by

$$C_{10} = \begin{bmatrix} 8.5588\times10^{-10} & 9.9413\times10^{-10} & 1.1324\times10^{-9} & 1.9883\times10^{-9} \end{bmatrix}^T$$

Consistency of the HBDF

Lambert (1973), explained that consistency controls the magnitude of the local truncation error while zero stability controls the manner in which the error is propagated at each step of the calculation.

Definition 2 (Lambert, 1973)

A LMM is said to be consistent if its order $p \geq 1$

According to Definition 2, the HBDF is consistent.

Zero-Stability of the HBDF

Definition 3 (Dahlquist, 1963)

A LMM is said to be zero-stable if the first characteristic polynomial $\Pi(r)$ satisfies $|r_z| \leq 1$ and if every root satisfying $|r_z| = 1$ have multiplicity not be greater than two. In order to find the zero-stability of HBDF, we only consider the first characteristic polynomial of the method according to Definition 3 as follows,

$$\Pi(r) = \left| r\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \right| = r^3(r-1)$$

which implies $r = 0, 0, 0, 1$. Hence, the HBDF is zero-stable since $|r_z| \leq 1$.

Convergence of the HBDF

Convergence is an essential property that every acceptable LMM must possess. According to Dahlquist (1963), consistency and zero-stability are the necessary conditions for the convergence of any numerical method.

Theorem 1 (Dahlquist, 1963)

The consistency and zero stability are sufficient condition for linear multistep method to be convergent. Since the HBDF is consistent and zero-stable, it implies that the method is convergent for all points.

Region of Absolute Stability of the HBDF

The absolute stability region consists of the set of points in the complex plane outside the enclosed figure. The absolute stability region of backward difference formulae is obtained using Dahlquist (1963) and is shown below.

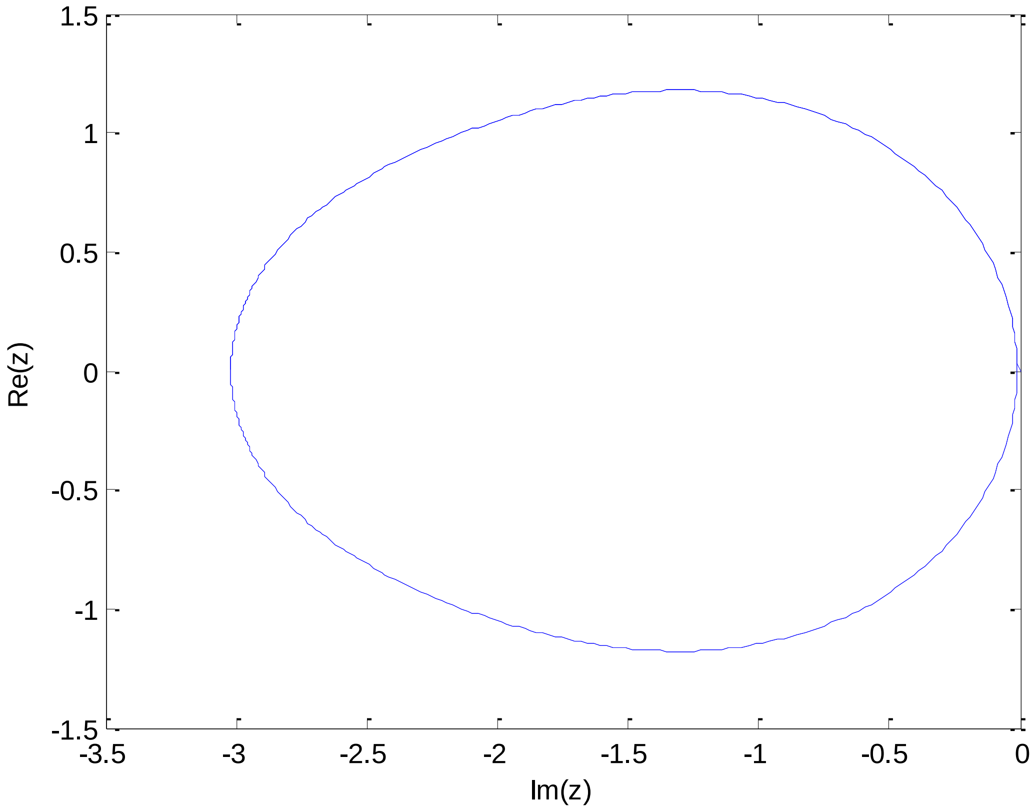

Figure 1: Absolute Stability Region of the HBDF

Numerical Experiments

To illustrate the performance of our proposed method, we will compare their performance with the existing methods. The problems considered are the ones solved by Skwame *et. al.* (2017a), Skwame, Kumleng and Bakari (2017b) and Tumba, Sabo and Hamadina (2018).

Problem 1

Consider the stiff system

$$y_1' = 198y_1 + 199y_2 \quad y_1(0) = 1$$

$$y_2' = -398y_1 - 399y_2 \quad y_2(0) = -1, \quad h = 0.1$$

with the exact Solution

$$y_1(x) = e^{-x}$$

$$y_2(x) = -e^{-x}$$

Table 1: Comparison of the absolute error of the new HBDF with those of Skwame, Kumleng and Bakari (2017b) and Skwame *et al.*, (2017a)

x	*Absolute errors in of Skwame, Kumleng and Bakari (2017b)* $K=2$ *and* $p=6$		*Absolute errors in of Skwame, et al., (2017a)* $K=1$ *and* $p=10$		*Absolute error in HBDF* $K=2$ *and* $p=10$	
	$y_1(x)$	$y_2(x)$	$y_1(x)$	$y_2(x)$	$y_1(x)$	$y_2(x)$
0.1	3.61×10^{-7}	3.60×10^{-7}	2.60×10^{-6}	2.60×10^{-6}	3.90×10^{-9}	2.90×10^{-9}
0.2	3.21×10^{-7}	3.30×10^{-7}	2.42×10^{-6}	2.42×10^{-6}	1.62×10^{-8}	1.52×10^{-9}
0.3	6.28×10^{-7}	3.27×10^{-7}	2.18×10^{-6}	2.18×10^{-6}	1.91×10^{-8}	1.84×10^{-8}
0.4	5.65×10^{-7}	5.65×10^{-7}	3.90×10^{-6}	3.90×10^{-6}	2.78×10^{-8}	2.70×10^{-8}
0.5	6.69×10^{-7}	6.68×10^{-7}	3.58×10^{-6}	3.58×10^{-6}	2.91×10^{-8}	2.84×10^{-8}
0.6	6.03×10^{-7}	6.02×10^{-7}	3.23×10^{-6}	3.23×10^{-6}	3.46×10^{-8}	3.39×10^{-8}
0.7	5.92×10^{-7}	5.92×10^{-7}	4.35×10^{-6}	4.35×10^{-6}	3.44×10^{-8}	3.38×10^{-8}
0.8	5.36×10^{-7}	5.37×10^{-7}	3.97×10^{-6}	3.97×10^{-6}	3.78×10^{-8}	3.30×10^{-8}
0.9	7.38×10^{-7}	7.38×10^{-7}	3.59×10^{-6}	3.59×10^{-6}	3.70×10^{-8}	3.65×10^{-8}
1.0	6.70×10^{-7}	6.70×10^{-7}	4.31×10^{-6}	4.30×10^{-6}	3.88×10^{-8}	3.84×10^{-8}

Problem 2

Consider the stiff system

$$y_1^1 = -8y_1 + 7y_2\,;\, y_1(0) = 1$$
$$y_2^1 = 42y_1 - 43y_2\,;\, y_2(0) = 8$$

with the exact solution

$$y_1(x) = 2e^{-x} - e^{-50x}$$
$$y_2(x) = 2e^{-x} - 6e^{-50x}$$

Table 2: Comparison of the absolute error of the new HBDF with those of Tumba, Sabo and Hamadina (2018) and Skwame *et. al.* (2017a)

x	*Error in Tumba, Sabo and Hamadina (2018)* $K=1$ *and* $p=8$		*Error in Skwame et. al. (2017a)* $K=1$ *and* $p=10$		*Error in HBDF* $K=2$ *and* $p=10$	
	$y_1(x)$	$y_2(x)$	$y_1(x)$	$y_2(x)$	$y_1(x)$	$y_2(x)$
0.1	2.36×10^{-4}	8.23×10^{-2}	1.32×10^{-6}	8.10×10^{-2}	3.82×10^{-5}	8.11×10^{-2}
0.2	3.26×10^{-6}	1.32×10^{-1}	1.90×10^{-8}	5.50×10^{-4}	2.22×10^{-4}	1.88×10^{-3}
0.3	2.60×10^{-8}	3.95×10^{-6}	4.00×10^{-9}	3.70×10^{-6}	1.51×10^{-6}	1.27×10^{-5}
0.4	5.00×10^{-9}	3.20×10^{-8}	4.00×10^{-9}	2.10×10^{-8}	7.00×10^{-8}	4.40×10^{-7}
0.5	8.00×10^{-9}	7.00×10^{-9}	2.00×10^{-9}	3.00×10^{-9}	1.00×10^{-9}	3.00×10^{-9}
0.6	8.00×10^{-9}	6.00×10^{-9}	3.00×10^{-9}	2.00×10^{-9}	0	2.00×10^{-9}
0.7	7.20×10^{-9}	8.40×10^{-9}	4.50×10^{-9}	2.90×10^{-9}	3.00×10^{-10}	1.00×10^{-10}
0.8	8.20×10^{-9}	7.60×10^{-9}	4.10×10^{-9}	3.70×10^{-9}	2.00×10^{-10}	1.50×10^{-9}
0.9	8.40×10^{-9}	8.50×10^{-9}	4.60×10^{-9}	4.00×10^{-9}	4.00×10^{-10}	1.00×10^{-10}
1.0	8.50×10^{-9}	8.00×10^{-9}	4.80×10^{-9}	4.60×10^{-9}	3.00×10^{-10}	1.30×10^{-9}

Problem 3

Consider the stiff system

$$y_1^1 = -y_1 + 95y_2\,;\, y_1(0) = 1$$

$$y_2^1 = -y_1 - 97y_2\,;\, y_1(0) = 1$$

with the exact Solution

$$y_1(x) = \frac{95}{47}e^{-2x} - \frac{48}{47}e^{-96x}$$

$$y_2(x) = \frac{48}{47}e^{-96x} - \frac{1}{47}e^{-2x}$$

Table 3: Comparison of the absolute error of the new HBDF with that of Skwame *et. al.* (2017a)

x	*Error in* Skwame *et. al.* (2017a) $K=1\,and\;p=10$		*Error in HBDF* $K=2\,and\;p=10$	
	$y_1(x)$	$y_2(x)$	$y_1(x)$	$y_2(x)$
0.1	1.74×10^{-4}	1.74×10^{-4}	7.73×10^{-4}	7.73×10^{-4}
0.2	5.40×10^{-8}	5.30×10^{-8}	7.74×10^{-3}	7.74×10^{-3}
0.3	1.00×10^{-9}	4.00×10^{-11}	6.38×10^{-6}	6.39×10^{-6}
0.4	2.30×10^{-9}	3.50×10^{-11}	5.87×10^{-5}	5.87×10^{-5}
0.5	2.20×10^{-9}	3.10×10^{-11}	4.65×10^{-8}	4.84×10^{-8}
0.6	1.80×10^{-9}	2.70×10^{-11}	4.42×10^{-7}	4.45×10^{-7}
0.7	1.60×10^{-9}	2.20×10^{-11}	1.60×10^{-9}	3.47×10^{-10}
0.8	1.40×10^{-9}	2.00×10^{-11}	1.20×10^{-9}	3.35×10^{-9}
0.9	1.20×10^{-9}	1.60×10^{-11}	1.80×10^{-9}	1.60×10^{-11}
1.0	9.00×10^{-10}	1.40×10^{-11}	2.00×10^{-9}	8.00×10^{-12}

It is obvious from the results displayed in the Tables 1, 2 and 3 that the new HBDF performs better than the existing methods with which we compared our results. Numerical results obtained using the proposed new HBDF show that it is the method is reliable for the solutions of stiff problems and compares favorably with existing ones.

Conclusion

The approach adopted for the derivation of the HBDF involves interpolation and collocation at appropriate selected points. The proposed order ten HBDF for general second order ODEs was found to be consistent, zero-stable and convergent. It also performed better than the methods with which we compared our results with.

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