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Construction and Implementation of Hybrid Backward Differentiation Formulas for the Solution of Second Order Differential Equations.

U. Mohammed[1] and R. B. Adeniyi[2]

[1]Department of Mathematics and Statistics, Federal University of Technology, Minna, Niger State, Nigerian. E-mail: digitalumar@yahoo.com
[2]Department of mathematics, University of Ilorin, Ilorin, Nigeria. E-mail: raphade@unilorin.edu.ng.

Abstract

In this paper, we propose a family of Hybrid Backward Differentiation Formulas (HBDF) for direct solution of general second order Initial Value Problems (IVPs) of the form $y''=f\left(x,y,y'\right)$. The method is derived by the interpolation and collocation of the assumed approximate solution and it's second derivative at $x=x_{n+j}$, $j=1,2,.....k-1$ and $x=x_{n+k}$ respectively, where k is the step number of the methods. The interpolation and collocation procedures lead to a system of (k+1) equations, which are solved to determine the unknown coefficients. The resulting coefficients are used to construct the approximate continuous solution from which the Multiple Finite Difference Methods (MFDMs) are obtained and simultaneously applied to provide the direct solution to IVPs. Two specific methods for k=2 and k=3 are used to illustrate the process. Numerical examples are given to show the efficiency of the method.

Keywords: Hybrid method, Backward Differentiation Formulas, Collocation, Interpolation, Second Order, Multiple Finite Difference.

1.0 Introduction

Many scientific and engineering problems are described using apparatus of Ordinary Differential Equations (ODEs), where the analytic solution is unknown. Much research has been done by the scientific community on developing numerical methods which can provide an approximate solution of the original ODE. In recent years many review articles and books have appeared on numerical methods for integrating ODEs, particularly in stiff cases [1]. Stiff problems are very common problems in many fields of the applied sciences: control theory, biology, chemical engineering processes, electrical networks, fluid dynamics, plastic deformation etc.
Most of numerical methods for solving Initial Value Problems (IVPs) for ODEs will become unbearably slow when the ODEs are stiff. The most popular multistep methods families for stiff ODEs are formed by the Backward Differentiation Formulae (BDF or Gear methods) methods, Rosenbrock methods, implicit or diagonally implicit Runge-Kutta methods [1-3]. In this paper we are suggested a construction of two and three step HBDF method, it is self-starting and can be applied for the numerical solution of IVPs (Cauchy problem) for second-order ODEs. Development of HybridBackwardDifferentialFormulas Methods (HBDF) for solving ODEs can be generated using different methods.We use the collocation technique for the construction of implicit HBDF.
Block methods for solving ODEs have initially been proposed by Milne [4].The Milne's idea of proceeding in blocks was developed by Rosser [5] for Runge-Kutta method. Also block Backward Differentiation Formulas (BDF) methods are discussed and developed by many researchers [6-14]. The method of collocation and interpolation of the power series approximate solution to generate continuous LMM has been adopted by many researchers among them are [15-16]

Corresponding author:U. MohammedE-mail: digitalumar@yahoo.com,Tel.: +2347032159609

The paper is presented as follows: In section 2, we discuss the basic idea behind the algorithm and obtain a continuous representation $Y(x)$ for the exact solution $y(x)$ which is used to generate members of the block method for solving IVPs. In section 3, we briefly discuss the order and error constant and convergence analysis of the method. Finally, we present numerical results and concluding remarks.

2.0 Development of Method

The mathematical formulation of physical phenomena in science and engineering often leads to initial value problems of the form:

$$y'' = f(x, y', y), \; y(a) = y_0 \;, \; y'(a) = \eta_0 \tag{1}$$

We seek an approximation of the form

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

Where $x \in [a,b], \ell_j$ are unknown coefficients to be determined and $1 \le r \prec k$ and $s \succ 0$ are the number of interpolation and collocation points respectively. We then construct our continuous approximation by imposing the following conditions

$$Y(x) = y_{n+j,} \; j = 0,1,2,...,.k-1 \tag{3}$$

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

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

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 ℓ_j into equation (2). After some manipulation, the continuous method is expressed as

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

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

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

$$Y'(x) = \delta(x) \tag{7}$$

$$Y'(a) = \delta_0 \tag{8}$$

2.1 Specification of Methods

2.1.1 Two Step Methods with one- off -step point at interpolation.

To derive these methods, we use Eq.(5) to obtained a continuous 2-step HBDF method with the following specification : r=3,s=1,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:

$$y(x) = \alpha_0 y_n + \alpha_1 y_{n+1} + \alpha_{\frac{3}{2}} y_{n+\frac{3}{2}} + h^2 \beta_2 f_{n+2} \tag{9}$$

where

$$\alpha_0 = 1 - \frac{41}{21} t + \frac{8}{7} t^2 - \frac{4}{21} t^3$$

$$\alpha_1 = \frac{27}{7} t - \frac{24}{7} t^2 + \frac{4}{7} t^3$$

$$\alpha_{\frac{3}{2}}=-\frac{40}{21}t+\frac{16}{7}t^2-\frac{8}{21}t^3$$

$$\beta_2=\frac{1}{14}\left(3t-5t^2+2t^3\right)$$

Evaluating (9) at $x=x_{n+2}$ yields Hybrid Two step implicit method

$$y_{n+2}=\frac{1}{7}y_n-\frac{10}{7}y_{n+1}+\frac{16}{7}y_{n+\frac{3}{2}}+\frac{1}{7}h^2f_{n+2} \qquad (10)$$

Taking the second derivative of equation (9), thereafter, evaluating the resulting continuous polynomial solution at $x=x_{n+\frac{3}{2}}$ we generate additional methods

$$y_{n+\frac{3}{2}}=-\frac{1}{2}y_n+\frac{3}{2}y_{n+1}+\frac{7}{8}h^2f_{n+\frac{3}{2}}-\frac{1}{2}h^2f_{n+2} \qquad (11)$$

Since our method is design to simultaneously provide the values of $y_{n+1},y_{n+\frac{3}{2}},y_{n+2}$ at a block point $x_{n+1},x_{n+\frac{3}{2}},x_{n+2}$, the two equations (10)-(11) are not sufficient to provide the solution for three unknown $y_{n+1},y_{n+\frac{3}{2}},y_{n+2}$. Thus, we obtain an additional method from (8), given by $42h\delta_0+82y_0-162y_1+80y_{\frac{3}{2}}=9h^2f_2$ (12)

The derivatives are obtained from (7) by imposing that $\delta\left(x_{n+\mu}\right)=\delta_{n+\mu},\mu=\{j,v\},\ j=0,...2,$ thus, we have

$$h\delta_{n+1}=-\frac{5}{21}y_n-\frac{9}{7}y_{n+1}+\frac{32}{21}y_{n+\frac{3}{2}}-\frac{1}{14}h^2f_{n+2}$$

$$h\delta_{n+\frac{3}{2}}=\frac{4}{21}y_n-\frac{18}{7}y_{n+1}+\frac{50}{21}y_{n+\frac{3}{2}}+\frac{3}{28}h^2f_{n+2}$$

$$h\delta_{n+2}=\frac{1}{3}y_n-3y_{n+1}+\frac{8}{3}y_{n+\frac{3}{2}}+\frac{1}{2}h^2f_{n+2}$$

2.1.2 Three Step Methods with one- off -step point at interpolation.

To derive this methods, we use Eq.(5) to obtain a continuous 3-step HBDF method with the following specification : r=4,s=1,*k*=3. We also express and $\beta_k\left(x\right)$ as a $\alpha_j(x),\alpha_\mu(x)$ functions of t, where $t=\dfrac{x-x_n}{h}$ to obtain the continuous form as follows

$$y\left(x\right)=\alpha_0y_n+\alpha_1y_{n+1}+\alpha_2y_{n+2}+\alpha_{\frac{5}{2}}y_{n+\frac{5}{2}}+h^2\beta_3f_{n+3} \qquad (13)$$

where

$$\alpha_0=1-\frac{43}{20}t+\frac{63}{40}t^2-\frac{19}{40}t^3+\frac{1}{20}t^4$$

$$\alpha_1=\frac{185}{42}t-\frac{141}{28}t^2+\frac{155}{85}t^3-\frac{3}{14}t^4$$

$$\alpha_2=-\frac{125}{28}t+\frac{405}{56}t^2-\frac{177}{56}t^3+\frac{11}{28}t^4$$

$$\alpha_{\frac{5}{2}} = \frac{232}{105}t - \frac{132}{35}t^2 + \frac{188}{105}t^3 - \frac{8}{35}t^4$$

$$\beta_3 = \frac{1}{56}\left(-10 + 19t^2 - 11t^3 + 2t^4\right)$$

Evaluating (13) at $x = x_{n+3}$ yields Hybrid Three step implicit method

$$y_{n+3} = -\frac{1}{20}y_n + \frac{5}{14}y_{n+1} - \frac{51}{28}y_{n+2} + \frac{88}{35}y_{n+\frac{5}{2}} + \frac{3}{28}h^2 f_{n+3} \quad (14)$$

Taking the second derivative of equation of equation (13), thereafter, evaluating the resulting continuous polynomial solution at $x = x_{n+2} x = x_{n+\frac{5}{2}}$ we generate two additional methods

$$y_{n+2} = -\frac{7}{215}y_n + \frac{50}{129}y_{n+1} + \frac{416}{645}y_{n+\frac{5}{2}} - \frac{28}{129}h^2 f_{n+2} + \frac{1}{129}h^2 f_{n+3} \quad (15)$$

$$y_{n+\frac{5}{2}} = \frac{63}{608}y_n - \frac{215}{304}y_{n+1} + \frac{975}{608}y_{n+2} + \frac{35}{76}h^2 f_{n+\frac{5}{2}} - \frac{115}{608}h^2 f_{n+3} \quad (16)$$

Since our method is design to simultaneously provide the values of $y_{n+1}, y_{n+2}, y_{n+\frac{5}{2}}, y_{n+3}$ at a block point $x_{n+1}, x_{n+2}, x_{n+\frac{5}{2}}, x_{n+3}$, the three equations (14)-(16) are not sufficient to provide the solution for three unknown $y_{n+1}, y_{n+2}, y_{n+\frac{5}{2}}, y_{n+3}$. Thus, we obtain an additional method from (8), given by

$$420h\delta_0 + 903y_0 - 1850y_1 + 1875y_2 - 928y_{\frac{5}{2}} = -75h^2 f_3 \quad (17)$$

The derivatives are obtained from (7) by imposing that $\delta\left(x_{n+\mu}\right) = \delta_{n+\mu}, \mu = \{j, v\}, j = 0,\ldots 3,$ thus, we have

$$h\delta_{n+1} = -\frac{9}{40}y_n - \frac{83}{84}y_{n+1} + \frac{117}{56}y_{n+2} - \frac{92}{105}y_{n+\frac{5}{2}} + \frac{3}{56}h^2 f_{n+3}$$

$$h\delta_{n+2} = \frac{1}{20}y_n - \frac{19}{42}y_{n+1} - \frac{25}{28}y_{n+2} + \frac{136}{105}y_{n+\frac{5}{2}} - \frac{1}{28}h^2 f_{n+3}$$

$$h\delta_{n+\frac{5}{2}} = -\frac{9}{160}y_n + \frac{145}{336}y_{n+1} - \frac{675}{224}y_{n+2} + \frac{277}{105}y_{n+\frac{5}{2}} + \frac{15}{224}h^2 f_{n+3}$$

$$h\delta_{n+3} = -\frac{1}{8}y_n + \frac{73}{84}y_{n+1} - \frac{223}{56}y_{n+2} + \frac{68}{21}y_{n+\frac{5}{2}} + \frac{23}{56}h^2 f_{n+3}$$

3.0 Error Analysis and Zero Stability

Following [15,17] we define the local truncation error associated with the conventional form of (5) to be the linear difference operator

$$L\left[y(x);h\right] = \sum_{j=0}^{k}\left\{\alpha_j y(x+jh)\right\} + \alpha_v y(x+vh) + h^2\beta_v y''(x+jh) \quad (18)$$

Assuming that y(x) is sufficiently differentiable, we can expand the terms in (18) as a Taylor series about the point x to obtain the expression

$$L\left[y(x);h\right] = C_0 y(x) + C_1 hy' + \ldots, + C_q h^q y^q(x) + \ldots, \quad (19)$$

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

$$C_0 = \sum_{j=0}^{k} \alpha_j ,$$

$$C_1 = \sum_{j=1}^{k} j\alpha_j ,$$

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$$.C_q = \left[\frac{1}{q!} \sum_{j=1}^{k} j^q \alpha_j - q(q-1) \sum_{j=1}^{k} j^{q-2} \beta_j \right].$$

According to [18], method (5) has order p if

$$C_0 = C_1 = ... = C_P = C_{P+1} = 0, \quad C_{P+2} \neq 0$$

Therefore, C_{p+2} is the error constant and $C_{p+2} h^{p+2} y^{(p+2)}(x_n)$ the principal local truncation error at the point x_n. It is establish from our calculations that the HBDF have higher order and relatively small error constants as displayed in the Table 1.

In order to analyze the methods for zero stability, we normalize the HBDF schemes and write them as a block method from which we obtain the first characteristic polynomial $\rho(R)$ given by

$$\rho(R) = \det\left(RA^{(0)} - A^{(1)} \right) = R^k (R-1) \tag{20}$$

Where $A^{(0)}$ is the identity matrix of dimension *k*+1, $A^{(1)}$ is the matrix of dimension *k*+1

Case *k*=2. It is easily shown that (10)-(12) are normalized to give the first characteristic polynomial $\rho(R)$ given by

$$\rho(R) = \det\left(RA^{(0)} - A^{(1)} \right) = R^2 (R-1)$$

Where $A^{(0)}$ an identity matrix of is dimension three and $A^{(1)}$ is a matrix of dimension three given by

$$A^{(1)} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix}$$

Case *k*=3. It is easily shown that (14)-(17) are normalized to give the first characteristic polynomial $\rho(R)$ given by

$$\rho(R) = \det\left(RA^{(0)} - A^{(1)} \right) = R^2 (R-1)$$

Where $A^{(0)}$ an identity matrix of is dimension four and $A^{(1)}$ is a matrix of dimension four given by

$$A^{(1)} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Following [15] the block method by combining k+1 HBDF is zero-stable, since from (20), $\rho(R) = 0$ satisfy $|R_j| \leq 1 \ j = 1...,k$ and for those roots with $|R_j|$=1, the multiplicity does not exceed 2. The block method by combining k+1 HBDF is consistent since HBDF have order $P > 1$. According to [18], we can safely ascertain the convergence of HBDF method.

Table 1:Order and Error Constants For the HBDF methods.

Step number	Method	order	Error constant
2	(10)	2	$-\frac{1}{24}$
	(11)	2	$-\frac{21}{64}$
	(12)	2	$-\frac{63}{8}$
3	(14)	3	$-\frac{23}{1120}$
	(15)	3	$-\frac{107}{24}$
	(16)	3	$-\frac{641}{24}$
	(17)	3	$-\frac{535}{8}$

4.0 Numerical Example

The HBDF methods are implemented as simultaneous numerical integration for IVPs without requiring starting values and predictors. We proceed by explicitly obtaining initial conditions at x_{n+k} , n=0,k,….,N-k using the computed values $Y\left(x_{n\_k}\right)=y_{n+k}$ and $\delta\left(x_{n\_k}\right)=\delta_{n+k}$ over sub-intervals $\left[x_0,x_k\right],...,\left[x_{N-K},x_N\right]$ which do not overlap. We give examples to illustrate the efficiency of the methods.

We report here a numerical example taken from the literature.

Problem [19]

$$y''+1001y'+1000y=0,\ y(0)=1, y'(0)=-1, h=0.1$$

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

Table 2: Showing Exact solutions and the computed results from the proposed HBDF methods

x	Exact Solution	K=2	K=3
0	1	1	1
0.1	0.9048374180	0.9048343762	0.9048371727
0.2	0.8187307531	0.8187335879	0.8187308287
0.3	0.7408182207	0.7408166016	0.7408181387
0.4	0.6703200460	0.6703216772	0.6703198322
0.5	0.6065306597	0.6065291218	0.6065307224
0.6	0.5488116361	0.5488131391	0.5488115690
0.7	0.4965853038	0.4965840964	0.4965851435
0.8	0.4493289641	0.4493301541	0.4493290111
0.9	0.4065696597	0.4065686593	0.4065696088
1.0	0.36787944	0.3678804248	0. 3678794425

Table 3: Comparing the absolute errors for two step and three step (HBDF) to errors in [19] for problem 1

x	Error in K=2 (HBDF)	Error in K=2 (BDF) [19]	Error in K=3 (HBDF)	Error in K=3(BDF) [19]
0	0.000000000E+00	0.000000000E+00	0.000000000E+00	0.000000000E+00
0.1	3.041800000E-06	2.940180000E-04	2.453000000E-07	1.111124000E-05
0.2	2.834800000E-06	5.571550000E-04	7.560000004E-08	5.749050000E-05
0.3	1.619100000E-06	7.512790000E-04	8.200000001E-08	9.210130000E-05
0.4	1.631200000E-06	9.202740000E-04	2.137999999E-07	4.078390000E-05
0.5	1.537900000E-06	10.29514000E-04	6.270000008E-08	2.530190000E-05
0.6	1.503000000E-06	11.26415000E-04	6.710000000E-08	4.725860000E-05
0.7	1.207400000E-06	11.80252000E-04	1.603000000E-07	1.893470000E-05
0.8	1.190000000E-06	12.27376000E-04	4.700000000E-08	4.288120008E-05
0.9	1.000400000E-06	12.42326000E-04	5.089999999E-08	7.966800000E-05
1.0	9.848000000E-07	12.54553000E-04	2.499999985E-09	2.941190000E-05

Problem 2

$$y'' + y = 0,\; y(0) = 1, y'(0) = 1, h = 0.1$$

Exact Solution $y(x) = \cos(x) + \sin(x)$

Table 4: Showing exact solutions and the computed results from the proposed methods for problem 2

x	Exact Solution	K=2	K=3
0	1	1	1
0.1	1.094837582	1. 094781733	1.094844138
0.2	1.178735909	1.178587196	1.178753798
0.3	1.250856696	1.250645384	1.250886052
0.4	1.310479336	1.310165070	1.310511922
0.5	1.357008100	1.356627096	1.357046032
0.6	1.389978088	1.389488483	1.390021138
0.7	1.409059874	1.408502167	1.409102595
0.8	1.414062800	1.413395513	1.414104578
0.9	1.404936878	1.404202948	1.404977272
1.0	1.38177329	1.380933499	1.381809897

Table 5: Comparing the absolute errors in new methods for problem 2

x	Error in K=2	Error in K=3
0	0.000000000E+00	0.000000000E+00
0.1	5.584900000E-05	6.556000000E-06
0.2	1.487130000E-04	1.788900000E-05
0.3	2.113120000E-04	2.935600000E-05
0.4	3.142660000E-04	3.258600000E-05
0.5	3.810040000E-04	3.793200000E-05
0.6	4.896050000E-04	4.305000000E-05
0.7	5.577070000E-04	4.272100000E-05
0.8	6.672870000E-04	4.177800000E-05
0.9	7.339300000E-04	4.039400000E-05
1.0	8.397910000E-04	3.660700000E-05

5.0 Conclusion

In this paper, we suggested and implemented new, more general versions of the two and three Step Block Hybrid Backward Differential Formula method.

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