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DERIVATION AND ANALYSIS OF BLOCK IMPLICIT HYBRID BACKWARD DIFFERENTIATION FORMULAE FOR STIFF PROBLEMS

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Abstract

The Hybrid Backward Differentiation Formula (HBDF) for the case $k = 3$ was reformulated into continuous form using the idea of multistep collocation. The continuous form was evaluated at some grid and off grid points which gave rise to discrete schemes employed as block methods for direct solution of first order Ordinary Differential Equation $y' = f(x, y)$. The requirement of a starting value and the overlap of solution model which are associated with conventional Linear Multistep Methods were eliminated by this approach. A convergence analysis of the derived hybrid schemes to establish their effectiveness and reliability is presented. Numerical example carried out on stiff problem further substantiates their performance.

1. Introduction

We consider the Initial Value Problem of the form:

$$y' = f(x, y)\ y(x_0) = y_0 \tag{1}$$

Where the solution y is assumed to be a differentiable function on an interval $[x_0, b], b < \infty$. Many methods for solving (1) exists, one particular method is the

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Linear Multistep Method. Linear Multistep Methods require less evaluation of the derivative function f than one step methods in the range of integral $[x_0, b]$. For this reason they have been very popular and important for solving (1) numerically. But these methods have certain limitations such as the overlap of solution models and the requirement of a starting value. Other limitations include they yield the discrete solution values $y_1, \ldots, y_N$ hence uneconomical for producing dense output. A continuous formulation is desirable in this respect. The collocation method is probably the most important numerical procedure for the construction of continuous methods (see [10], [12], [13], [14]).
In this research paper, we derived the Block Hybrid Backward Differentiation Formulae (BHBDF) for step ($k = 3$). The block methods were used to solve (1) directly without the need of a starting value. Their performances were compared with the analytical solution to the problem (see [1], [6], [7], [15], [16] and [17]).

2. The Multistep Collocation (CMM) Method

Lambert [8], [9] adopted the Continous Finite Difference (CFD) approximation method by the idea of interpolation and collocation. Later, Lie [10], Onumanyi [12], [13] referred to it as Multistep Collocation (MC). The method is presented below:

$$\underline{a} = (a_0, a_1, a_2, \ldots, a_{(t+m-1)})^T, \varphi(x) = (\varphi_0(x), \varphi_1(x), \ldots, \varphi_{(t+m-1)})^T \quad (2)$$

where $a_r, r = 0, \ldots, t+m-1$ are undetermined constants, $\varphi_r(x)$ are specified basis functions, T denotes transpose of, t denotes the number of interpolation points and m denotes the number of distinct collocation points. We consider a continuous approximation (interpolant) $Y(x)$ to $y(x)$ in the form:

$$y(x) = \sum_{r=0}^{t+m-1} a_r \varphi_r(x) = \underline{a}^T \varphi(x) \quad (3)$$

which is valid in the sub-intervals $x_n \leq x \leq x_{n+k}$, where $n = 0, k, \ldots, N-k$. The quantities $x_0 = a, x_N = b, k, m, n, t$ and $\varphi_r(x), r = 0, 1, ..., t+m-1$ are specified values. The constant co-efficient a_r of (3) can be determined using the conditions:

$$y(x_{n+j}) = y_{n+j},\ j = 0, 1, \ldots, t-1 \quad (4)$$

$$y'(\bar{x_j}) = f_{n+j}\ j = 0, 1, \ldots, m-1 \quad (5)$$

where

$$f_{n+j} = f(x_{n+j}, x_{n+j}) \quad (6)$$

The distinct collocation points $x_0, \ldots, x_(m-1)$, can be chosen freely from the set $[x_n, x_{n+k}]$. Equation (4), (5) and (6) are denoted by a single set of algebraic equations of the form:

$$D\underline{a} = \underline{F} \tag{7}$$

where

$$\underline{F} = (y_n, y_{n+1}...y_{n+t-1}, f_n, f_{n+1}, \ldots, f_{n+m-1})^T \tag{8}$$

$$\underline{a} = D^{-1}\underline{F} \tag{9}$$

where $\underline{D}$ is the non-singular matrix of dimension $(t+m)$ below:

$$\underline{D} = \begin{pmatrix} \varphi_0(x_n) & \cdots & \varphi_{t+m-1}(x_n) \\ \vdots & \vdots & \vdots \\ \varphi_(x_{n+t-1}) & \cdots & \varphi_{t+m-1}(x_{n+t-1}) \\ \varphi_0(\bar{x_0}) & \cdots & \varphi_{t+m-1}(\bar{x_0}) \\ \vdots & \vdots & \vdots \\ \varphi_0(\bar{x}_{m-1}) & \vdots & \varphi_{t+m-1}(\bar{x}_{m-1}) \end{pmatrix} \tag{10}$$

By substituting (9) into (3), we obtain the MC formula:

$$y(x) = F^T\zeta^T\varphi(x),\ x_n \leq x \leq x_{n+k}\ n = 0, k, \ldots, N-k \tag{11}$$

where

$$\zeta = D^{-1} = (c_{ij}), i, j = 1, ...t+m-1$$

$$\zeta = \begin{pmatrix} c_{11}, . & ..c_{1t} & c_{1,t+1} & c_{1,t+m} \\ . & . & . & . \\ c_{21}, . & ..c_{2t} & c_{2,t+1} & c_{2,t+m} \\ . & . & . & . \\ c_{t+m1}, . & ..c_{t+m,t} & c_{t+m,t+1} & ..c_{t+m,t+m} \end{pmatrix}$$

with the numerical elements denoted by $c_{ij},\ i, j = 1, ..., k+m$. By expanding $C^T\varphi(x)$ in (11) yields the following:

$$y(x) = (F)^T \begin{pmatrix} \sum_{r=0}^{t+m-1} C_{r+1,1\varphi_r(x)} \\ \sum_{r=0}^{t+m-1} C_{r+1,k+m\varphi_r(x)} \end{pmatrix} \tag{12}$$

$$y(x) = \sum_{j=0}^{t-1}\sum_{r=0}^{t+m-1} C_{r+1,j+1}\varphi_r(x) + \sum_{j=0}^{m-1} h \left(\sum_{r=0}^{k+m-1} \sum \frac{C_{r+1,j+1}}{h}\varphi_r(x)\right) f_{n+j} \tag{13}$$

$$y(x) = \sum_{j=0}^{t-1} \alpha_j(x) y_{n+j} + h\sum_{j=0}^{m-1} \beta_j(x) f_{n+j} \tag{14}$$

where we construct $\alpha_j(x)$ and $\beta_j(x)$ explicitly by

$$\alpha_j(x) = \sum_{r=0}^{t+m-1} C_{r+1,j+1}\varphi_r(x), j = 0, 1, ..., t-1 \tag{15}$$

$$\beta_j(x) = \sum_{r=0}^{k+m-1} \left(\frac{C_{r+1,j+1}}{h}\varphi_r(x)\right), j = 0, 1..., m-1 \tag{16}$$

a_r can be determined as follows:

$$y(x) = \left\{\sum_{j=0}^{t-1} \alpha_{j,r+1} y_{n+j} + h\sum_{j=0}^{m-1} \beta_{j,r+1} f_{n+j}\right\}\varphi_r(x) \tag{17}$$

For $K = 3$, the general form of the method upon addition of one off grid point is expressed as:

$$y(x) = \alpha_1(x)y_n + \alpha_2(x)y_{n+1} + \alpha_3(x)y_{n+2} + \alpha_4(x)y_{n+\frac{1}{2}} + h\beta_0(x)f_{n+3} \tag{18}$$

The matrix D of the proposed method is expressed as:

(19)

$$\begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 \\ 1 & (x_n+h) & (x_n+h)^2 & (x_n+h)^3 & (x_n+h)^4 \\ 1 & (x_n+2h) & (x_n+2h)^2 & (x_n+2h)^3 & (x_n+2h)^4 \\ 1 & (x_n+\frac{1}{2}h) & (x_n+\frac{1}{2}h)^2 & (x_n+\frac{1}{2}h)^3 & (x_n+\frac{1}{2}h)^4 \\ 0 & 1 & (2x_n+6h) & 3(x_n+3h)^2 & 4(x_n+3h)^3 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \end{pmatrix} = \begin{pmatrix} y_n \\ y_{n+1} \\ y_{n+2} \\ y_{n+\frac{1}{2}} \\ f_{n+3} \end{pmatrix}$$

i.e. $Da = F$

The matrix D in equation (19) which when solved by matrix inversion technique or Gaussian Elimination method will yield the continuous coefficients substituted in (18) to obtain continuous form of the three step block hybrid Backward Differentiation Formula (HBDF)o with one off step interpolation point.

$$\begin{aligned} y(x) = &\left(\frac{1}{134}\frac{134h^4 + 507x_nh^3 + 602x_n^2h^2 + 267x_n^3h + 38x_n^4}{h^4} - \frac{1}{134}\frac{507h^3 + 1204x_nh^2 + 801x_n^2h + 152x_n^3}{h^4}x\right. \\ &\left. + \frac{1}{134}\frac{602h^2 + 801x_nh + 228x_n^2}{h^4}x^2 - \frac{1}{134}\frac{267h + 152x_n}{h^4}x^3 + \frac{19}{67h^4}x^4\right)y_n \\ &+ \left(\frac{1}{67}\frac{x_n186h^3 + 517x_nh^2 + 316x_n^2h + 52x_n^3}{h^4} - \frac{2}{67}\frac{93h^3 + 517x_nh^2 + 474x_n^2h + 104x_n^3}{h^4}x\right. \\ &\left. + \frac{1}{67}\frac{517h^2 + 948x_nh + 312x_n^2}{h^4}x^2 - \frac{4}{67}\frac{79h + 52x_n}{h^4}x^3 + \frac{52}{67h^4}x^4\right)y_{n+1} \\ &+ \left(-\frac{1}{402}\frac{x_n460x_nh^2 + 393x_n^2h + 74x_n^3 + 141h^3}{h^4} + \frac{1}{402}\frac{920x_nh^2 + 1179x_n^2h + 296x_n^3 + 141h^3}{h^4}x\right. \end{aligned}$$

$$- \frac{1}{402}\frac{460h^2 + 1179x_nh + 444x_n^2}{h^4}x^2 + \frac{1}{402}\frac{393h + 296x_n}{h^4}x^3 + \frac{37}{201h^4}x^4\Bigg) y_{n+2}$$

$$+ \Bigg(\frac{-16}{201}x_n\frac{11x_n^3 + 72x_n^2h + 139x_nh^2 + 78h^3}{h^4} + \frac{32}{201}\frac{22x_n^3 + 108x_n^2h + 139x_nh^2 + 39h^3}{h^4}x$$

$$- \frac{16}{201}\frac{66x_n^2 + 216x_nh + 139h^2}{h^4}x^2 + \frac{-1}{67}\frac{8x_n + 7h}{h^3}\frac{64}{201}\frac{11x_n + 18h}{h^4}x^3 - \frac{176}{201h^4}x^4\Bigg) y_{n+\frac{1}{2}}$$

$$+ \Bigg(\frac{1}{67}\frac{x_n(2x_n^3 + 7x_n^2h + 7x_nh^2 + 2h^3)}{h^3} - \frac{1}{67}\frac{8x_n^3 + 21x_n^2h + 14x_nh^2 + 2h^3}{h^3}x$$

$$+ \frac{1}{67}\frac{12x_n^2 + 21x_nh + 7h^2}{h^3}x^2 - \frac{1}{67}\frac{8x_n + 7h}{h^3}x^3 + \frac{2}{67h^3}x^4\Bigg) f_{n+3} \tag{20}$$

Evaluating equation (20) at $x = x_{n+3}$ and its derivative at $x = x_{n+1}, x = x_{n+2}, x = x_{n+\frac{1}{2}}$ yields the following four discrete hybrid schemes which are used as block integrators:

$$\frac{225}{67}y_{n+1} - \frac{150}{67}y_{n+2} + y_{n+3} - \frac{192}{67}y_{n+\frac{1}{2}} = \frac{-50}{67}y_n + \frac{30}{67}hf_{n+3}$$

$$y_{n+1} + \frac{52}{324}y_{n+2} - \frac{448}{324}y_{n+\frac{1}{2}} = \frac{-72}{324}y_n + \frac{201}{324}hf_{n+1} + \frac{3}{324}hf_{n+3}$$

$$\frac{1476}{649}y_{n+1} - y_{n+2} - \frac{1088}{649}y_{n+\frac{1}{2}} = -\frac{261}{649}y_n - \frac{402}{649}hf_{n+2} + \frac{36}{649}hf_{n+3}$$

$$-\frac{2880}{1600}y_{n+1} + \frac{245}{1600}y_{n+2} + y_{n+\frac{1}{2}} = -\frac{1035}{1600}y_n - \frac{1608}{1600}hf_{n+\frac{1}{2}} + \frac{18}{1600}hf_{n+3} \tag{21}$$

Equation (21) constitute the members of a zero-stable implicit block integrators of order $(4,4,4,4)^T$ with $C_5 = \left[-\frac{15}{268}, \frac{41}{4020}, -\frac{97}{2680}, -\frac{79}{8576}\right]^T$ as the error constants respectively. To start the integration process with $n = 0$, we use (21) and this produces $y_1, y_{\frac{1}{2}}, y_2$ and y_3 simultaneously without the need for any starting method (predictor).

3. Stability Analysis

Following Fatunla [2], [3], [4], that defined the block method to be zero-stable provided the roots $R_{ij} = 1(1)k$ of the first characteristic polynomial $\rho(R)$ specified as:

$$\rho(R) = det\left|\sum_{i=0}^{k} A^{(i)}R^{k-i}\right| = 0 \tag{22}$$

satisfies $|R_j| \leq 1$, the multiplicity must not exceed 2.
The block methods proposed in equations (21) for $k = 3$ are put in the matrix equation form and for easy analysis the result was normalized to obtain:

$$A^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \; A^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{23}$$

The first characteristic polynomial of the block method is given by $\rho(R) = det(RA^0 - A^1)$. Substituting the A^0 and A^1 into the function above gives

$$\rho(R) = det\left[R\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}\right] \tag{24}$$

$$= det\begin{pmatrix} R & 0 & 0 & -1 \\ 0 & R & 0 & -1 \\ 0 & 0 & R & -1 \\ 0 & 0 & 0 & R-1 \end{pmatrix}$$

$$= R^2(R(R-1)) - 0 = 0 \Rightarrow R_1 = R_2 = R_3 = 0 \; or \; R_4 = 1$$

To determine the order and error constant, we consider the Taylor series expansion of
(25)

$$\left.\begin{aligned}
y_{n+\frac{1}{2}h} &= y\left(n+\tfrac{1}{2}\right) = y(n) + \tfrac{1}{2}hy'(n) + \frac{\left(\frac{1}{2}h\right)^2}{2!}y''(n) + \frac{\left(\frac{1}{2}h\right)^3}{3!}y'''(n)+,...,+\frac{\left(\frac{1}{2}h\right)^s}{s!}y^s(n) \\
y_{n+1} &= y_{n+h} = y(n) + hy'(n) + \frac{(h)^2}{2!}y''(n) + \frac{(h)^3}{3!}y'''(n) + \frac{(h)^4}{4!}y^{iv}(n)+,...,+\frac{(h)^s}{s!}y^s(n) \\
y_{n+2} &= y_{n+2h} = y(n) + 2hy'(n) + \frac{(2h)^2}{2!}y''(n) + \frac{(2h)^3}{3!}y'''(n) + \frac{(2h)^4}{4!}y^{iv}(n)+,...,+\frac{(2h)^s}{s!}y^s(n) \\
y_{n+3} &= y_{n+3h} = y(n) + 3hy'(n) + \frac{(3h)^2}{2!}y''(n) + \frac{(3h)^3}{3!}y'''(n) + \frac{(3h)^4}{4!}y^{iv}(n)+,...,+\frac{(3h)^s}{s!}y^s(n) \\
f_{\frac{1}{2}} &= y\left(n+\tfrac{1}{2}h\right) = y'(n) + \tfrac{1}{2}hy''(n) + \frac{\left(\frac{1}{2}h\right)^2}{2!}y''(n) + \frac{\left(\frac{1}{2}h\right)^3}{3!}y'''(n)+,...,+\frac{\left(\frac{1}{2}h\right)^{s-1}}{s-1!}y^s(n) \\
f_1 &= y_{n+h} = y'(n) + hy''(n) + \frac{(h)^2}{2!}y'''(n) + \frac{(h)^3}{3!}y^{iv}(n) + \frac{(h)^4}{4!}y^v(n)+,...,+\frac{(h)^{s-1}}{(s-1)!}y^s(n) \\
f_2 &= y_{n+2h} = y'(n) + 2hy''(n) + \frac{(2h)^2}{2!}y'''(n) + \frac{(2h)^3}{3!}y^{iv}(n) + \frac{(2h)^4}{4!}y^v(n)+,...,+\frac{(2h)^{(s-1)}}{(s-1)!}y^s(n) \\
f_3 &= y_{n+3h} = y'(n) + 3hy''(n) + \frac{(3h)^2}{2!}y'''(n) + \frac{(3h)^3}{3!}y^{iv}(n) + \frac{(3h)^4}{4!}y^v(n)+,...,+\frac{(3h)^{s-1}}{(s-1)!}y^s(n)
\end{aligned}\right\}$$

By substituting into each of equation (21), we have

$$\frac{225}{67}y_{n+1} - \frac{150}{67}y_{n+2} + y_{n+3} - \frac{192}{67}y_{n+\frac{1}{2}} + \frac{50}{67}y_n - \frac{30}{67}hf_{n+3} = -\frac{15}{268}h^5y^5,$$

the method is of order 4 and the error constant is $-\frac{15}{268}$.

$$y_{n+1}+\frac{52}{324}y_{n+2}-\frac{448}{324}y_n+\frac{1}{2}+\frac{72}{324}y_n-\frac{201}{324}hf_{n+1}-\frac{3}{324}hf_{n+3}=\frac{41}{324020}h^5y^5,$$

the method is of order 4 and the error constant is $\frac{41}{4020}$

$$\frac{1476}{649}y_{n+1}-y_{n+2}-\frac{1088}{649}y_(n+\frac{1}{2})+\frac{261}{649}y_n+\frac{402}{649}hf_{n+2}-\frac{36}{649}hf_{n+3}=-\frac{97}{2680}h^5y^5,$$

the method is of order 4 and the error constant is $-\frac{97}{2680}$

$$-\frac{2880}{1600}y_{n+1}+\frac{245}{1600}y_{n+2}+y_{n+1/2}+\frac{1035}{1600}y_n+\frac{1608}{1600}hf_{n+\frac{1}{2}}-\frac{18}{1600}hf_{n+3}=-\frac{79}{8576}h^5y^5,$$

the method is of order 4 and the error constant is $-\frac{79}{8576}$
From equation (25) the hybrid method is zero stable and consistent since (22) is satisfied and the order of the method $p = 4 > 1$(as shown above). And by [5]; the hybrid method is convergent.

4. Numerical Example

To illustrate the performance of our proposed methods we will compare their performance with analytical results. Consider the Initial Value Problem

$$y' = \lambda(y - x) + 1,\ y(0) = 1$$

The problem is stiff in nature for negative λ values and it has analytical solution $y(x) = e^{\lambda x} + x$.
The problem is solved with $\lambda = -5$,and $\lambda = -20$ and steplength $h = 0.01$ using the Block Hybrid Backward Difference Formulae(BHBDF) for $k = 3$.
Table 1: Proposed BHBDF for $k = 3, \lambda = -5$

N	X	$Exact\ Value$	$ApproxitionValue$	$Error$
0	0.00	1.000000000	1.000000000	0.000
1	0.01	0.961229424	0.96122943	6.000×10^{-9}
2	0.02	0.924837418	0.924837426	8.000×10^{-9}
3	0.03	0.890707976	0.890707978	2.000×10^{-9}
4	0.04	0.858730753	0.858730759	6.000×10^{-9}
5	0.05	0.828800783	0.828800791	8.000×10^{-9}
6	0.06	0.800818223	0.800818223	3.000×10^{-9}
7	0.07	0.774688089	0.774688096	6.280×10^{-9}
8	0.08	0.750320046	0.750329954	8.876×10^{-9}
9	0.09	0.727628151	0.727628155	4.395×10^{-9}
10	0.1	0.706530659	0.706530667	8.000×10^{-9}

Table 2: Proposed BHBDF for $k = 3, \lambda = -20$

N	X	$Exact\ Value$	$ApproxitionValue$	$Error$
0	0.00	1.000000000	1.000000000	0.000
1	0.01	0.828730753	0.828734704	3.951×10^{-6}
2	0.02	0.690320046	0.69032541	5.364×10^{-6}
3	0.03	0.578811636	0.578811514	1.220×10^{-7}
4	0.04	0.489328964	0.489331033	2.069×10^{-6}
5	0.05	0.417879441	0.417882303	2.862×10^{-6}
6	0.06	0.361194211	0.361194078	1.330×10^{-7}
7	0.07	0.316596963	0.316598044	1.081×10^{-6}
8	0.08	0.281896518	0.281898044	1.526×10^{-6}
9	0.09	0.255298888	0.255298778	1.100×10^{-7}
10	0.1	0.235335283	0.235335846	5.6300×10^{-7}

Remark

For accuracy and performance, the block method was compared with analytical solution and it produced a very good result.

5. Conclusion

We have derived the hybrid form of the Backward Differentiation Formulae (BDF) for k=3. The idea of Multistep Collocation (MC) was used to reformulate the derived hybrid formulae into continous form which were employed as block methods for direct solution of $y' = f(x, y)$. A convergence analysis of the discrete hybrid methods to establish their effectiveness and reliability was presented. The methods were tested on stiff IVP and shown to perform satisfactorily without the requirement of any starting method.

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