INT. J. NUM. MATHS. (2011) Vol. 6 No. 1 pp- 16-30

FULLY IMPLICIT THREE POINT BLOCK ACKWARD DIFFERENTIATION FORMULAE FOR SOLUTION OF FIRST ORDER INITIAL VALUE PROBLEMS

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ABSTRACT

In this paper we reformulate the three step backward differentiation formulae (BDF) into the continuous form. The process produces some schemes which are combined together to form the block method for an accurate and efficient parallel or sequential solution of ODE's. The suggested approach eliminates requirement for a starting value and the proposed method can handle stiff problem because of its A-stability property.

1.0 INTRODUCTION

Consider the initial value problems for the system/scalar ordinary differential equations (ODEs).

$$y' = f(x, y) \quad y(a) = y_0, a \le x \le b \tag{1.1}$$

In the literature, conventional linear multistep methods including hybrid ones have been made continuous through the idea of multistep collocation (MC),[see Lie and Norsett (1989), Onumanyi etal (1994), Onumanyi etal (1999), yusuph and Onumanyi(2002), and yahaya (2004)]. The continuous method[CM] produces piece-wise polynomial

keywords: Block Method, Parallels
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solutions over K-steps $[X_n, X_{n+k}]$ for the first order systems/scalar ODEs. Of note, is that the implicit CM interpolant (3.1) is not to be directly used as the numerical integrator, but the resulting discrete multistep method which is derived from it, is self starting and can be applied for direct parallel or sequential solutions of both the initial and boundary value problems.

This paper is part of research effort to reformulate for efficient and accurate use, the linear multistep methods in general and three- step block backward differentiation formulae (BDF) is considered here. The standard three step block differentiation formulae (BDF) (see Lambert 1973, 1991) method in discrete or continuous form requires starting value for initial value problems. Moreover, the continuous method does not allow for block formulation which could have eliminated the requirement for starting values. The continuous method with variant is presented using the matrix inversion technique with the following advantages.

(1.) Evaluating (3.3) At $x=x_{n+3}$, the standard three step block differentiation formulae (BDF) which is well Known was obtained but because of earlier identified drawbacks, the method is not porpular.

(2.) It allows the block formulation and therefore is self starting and for appropriate choice of k, overlap of solution model is eliminated.

Def1.1 A-Stable (Dahlqquist 1963)

A numerical method is said to be A-stable if its region of absolute stability contains, the whole of the left-hand half-plane Reh $\lambda < 0$.

Definition 1.2: $A(\alpha)$ stable (Widluid 1967) A numerical method is said to be $A(\alpha)$ $stable$ $\alpha \in (0, \pi/2)$ if its region of absolute stability contains the infinite wedge $w = [h\lambda \,|\, -\alpha < \pi - \arg h\lambda]$ it is said to be A (0)- stable if it is $A(\alpha)$ – stable for some (sufficiently small) $\alpha \in (0, \pi/2)$.

Definition 1.3

A block method is zero-stable provided the roof $\lambda_j, j = 1(1)s$ of the first characteristics polynomial $\rho(\lambda)$ specified as $\rho(\lambda) = det\left|\sum_{i=0}^{j} A^{(i)}\lambda^{(j-i)}\right| = 0$ satisfies $|\lambda_j| \le 1$ and for those roots with $|\lambda_j| = 1$ the multiplicity must not exceed two. The principal root of $\rho(\lambda)$ is denoted by $\lambda_1 = \lambda_2 = 1$

2.0 GENERAL MC LINKED TO CM INTERPOLANT

Let us first give a general description for the method of multistep collocation (MC) and its link to continuous multistep (CM) method for (1.1). in the equation (2.1), f is given and y is sought as

$$y = a_1\phi_1 + a_2\phi_2 + \dots\dots\dots + a_p\phi_p \quad (2.1)$$

Where

$a = (a_1, a_2 .... a_p)^T, \quad \phi = (\phi_1, \phi_2 .... \phi_p)^T$

$x_n \le x \le x_{n+k}$ Where $n = 0, k \ldots N - k$, and T denote Transpose of'

Equation (2.1) can be re-written as

$$y = (a_1, a_2 .... a_p)^T (\phi_1, \phi_2 .... \phi_p)^T \quad (2.2)$$

The unknown coefficients $a_1, a_2 .... a_p$ Are determined using respectively the

r(0<r<=k) interpolation conditions and the s>0 distinct collocation conditions, p=r+s as follows

$$\sum_{j=1}^{p} a_j \varphi_j(x_i) = y_i, \qquad (i = 1, ... r)$$

$$\sum_{j=1}^{p} \beta_j \varphi'_j(x_i) = f_i, \qquad (i = 1, ... r) \quad (2.3)$$

This is a system of p linear equations from which we can compute values for the unknown coefficients provided (2.3) is assumed non-singular, for the distinct points x_i and c_i the non-singular system is guaranteed (see proof in Yahaya 2004). We can write (2.3) as a single set of linear equations of the form

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

$$\underline{a} = \underline{\underline{D}}^{-1} \underline{F} \quad (2.4)$$

Where $\underline{F} = (y_1 y_2, \dots, y_r, f_1, f_2, \dots, f_s)^T$ (2.5)

Substituting the vector a, given by (2.4) and F by (2.5) into (2.2) gives

$$y = (y_1 . y_2 . \dots . y_r . f_1 . f_2 . \dots f_s) C^{T} (\phi_1 . \phi_2 \dots \phi_p)^T \quad (2.6)$$

Equation (2.6) is the continuous MC Interpolant C^T known explicitly in the form

$$\underline{\underline{C^T}}\phi = \begin{pmatrix} C_{11} & C_{21} \dots\dots & C_{p1} \\ C_{12} & C_{22} & C_{p2} \\ \vdots & \vdots & \vdots \\ C_{1r} & C_{2r} & C_{pr} \\ \vdots & \vdots & \vdots \\ C_{1p} & C_{2p} & C_{pp} \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_r \\ \vdots \\ \phi_p \end{pmatrix} \quad (2.7)$$

$$\underline{\underline{C^T}}\phi = \begin{pmatrix} \sum_{j=1}^{p} C_{ji\phi_j} \\ \vdots \\ \sum_{j=1}^{p} C_{jr\phi_j} \\ \sum_{j=1}^{p} C_{jr+1\phi_j} \\ \vdots \\ \sum_{j=1}^{p} C_{jp\phi_j} \end{pmatrix} = \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_2 \\ \beta_1 \\ \vdots \\ \beta_s \end{pmatrix} \quad (2.8)$$

$$F^T C^T \phi = (\alpha_1 y_1 + \alpha_2 y_2 + \dots\dots\dots + \alpha_r y_r + \beta_1 f_1 + \beta_2 f_2 + \dots\dots\dots + \beta_s f_s)$$

Or

$$F^T C^T \phi = \sum_{j=1}^{r} \alpha_j y_j + h_j \left(\sum_{j=1}^{s} \beta_j / h_j \, f_j \right) \tag{2.9}$$

Where, from (2.8)

$$\alpha_j = \sum_{q=i}^{p} C_{qi}\phi_j, \quad j = 1,\ldots,r$$

$$\beta_j / h_j = \sum_{q=i}^{p} \left[\frac{C_{qi+r}}{h_i} \right] \phi_j \quad j = 1,\ldots,s \tag{2.10}$$

Therefore,

$$y = \sum_{j=1}^{r} \alpha_j y_j + h_j \left(\sum_{j=1}^{s} \beta_j / h_j \right) f_j \tag{2.11}$$

Where $\alpha_j, \beta_j / h_j$ are given by (2.10). Hence (2.11) with (2.10) is the CM interpolant with constant step-size though it can be varied.

3.0 Derivation of the Present Methods

We propose an approximate solution to (1.1) in the form

$$y_p(x) = \sum_{j=0}^{m+t-1} a_j x^i, \; i = 0, (1)(m+t-1) \tag{3.1}$$

With $m = 1, t = 3$ and $p = m + t - 1$ also $a_j = j = 0.1.(m + t - 1)$ Are the parameters to be determined where p, is the degree of the polynomial interpolant of our choice. Specifically, we interpolate equation (3.1) at $\{x_n, x_{n+1}, x_{n-2}\}$ and collocate at x_{n-3} using the method described in section 2 of this paper; we obtain a continuous form for the solution $\bar{y}(x) = VC^T P(x)$, from the system of the equation in the matrix below.

The general form of the new method is expressed as;

$$y(x) = \alpha_0 y_n - \alpha_1 y_{n+1} + \alpha_2 y_{n+2} - \beta_0 f_{n-3} \quad (3.2)$$

The matrix D of the new method is expressed as:

$$\begin{pmatrix} 1 & x_n & x_n^2 & x_n^3 \\ 1 & x_{n+1} & x_{n+1}^2 & x_{n+1}^3 \\ 1 & x_{n+2} & x_{n+2}^2 & x_{n+2}^3 \\ 0 & 1 & 2x_{n+3} & 3x_{n+3}^2 \end{pmatrix} \quad (3.3)$$

Matrix D in equation (3.3) above, which can be solved by any matrix inversion techniques or Gaussian elimination method to obtain the values of the parameters $a_\gamma\, j == 0\,1\, m - t - 1$ and then substituting them into equation (3.1) give a scheme expressible in the form.

$$y_k(x) = \sum_{j=0}^{k-1} \alpha_j(x) y_{n+j} + h \sum_{j=0}^{k-2} \beta_j(x) f_{n+j} \quad (3.4)$$

If we now let k=3, after some manipulation we obtain a continuous form of solution.

$$y(x) = \left[\frac{-3(x-x_n)^3 + 20(x-x_n)^2 h - 39(x-x_n) h^2 + 22h^3}{22h^3} \right] y_n$$

$$\left[\frac{4(x-x_n)^3 - 23(x-x_n)^2 h + 30(x-x_n) h^2}{11h^3} \right] y_{n+1}$$

$$\left[\frac{-5(x-x_n)^3+26(x-x_n)^2h-21(x-x_n)h^2}{622\;h^4}\right]y_{n+2}$$

$$\left[\frac{(x-x_n)^3-3(x-x_n)^2h+2(x-x_n)h^2}{11\,h^2}\right]f_{n+3}$$

(3.5)

Evaluating (3.5) at $x=x_{n+3}$, we obtain

$$y_{n+3}=\frac{2}{11}y_n-\frac{9}{11}y_{n+1}+\frac{18}{11}y_{n+2}+\frac{6}{11}f_{n+3} \qquad (3.6)$$

This is the well known 3-step(BDF) method (see Lambert (1973), (1991)) of order three (3) with error constant

$E=-\frac{3}{22}h^5y^5$

In the same vein, its derivative is evaluated at point $x=x_{n+2}\ and\ x=x_{n+1}$ we obtain respectively

$$y_{n+2}=-\frac{5}{23}y_n+\frac{28}{23}y_{n+1}+\frac{22}{23}f_{n+2}-\frac{4}{23}hf_{n+3}$$

$$y_{n+1}=-y_n+2y_{n+2}-\frac{11}{4}f_{n+1}-\frac{1}{4}f_{n+3} \qquad (3.7)$$

equation (3.6) and (3.7) constitutee the member of a zero-stable block integrator of orders $(3,3,3)^T$ with

$C_4=\left(-\frac{3}{22}\ -\frac{17}{6}\ -\frac{7}{6}\right)$.

To start the IVP integration on the subinterval $[x_0, x_3]$.

We combine (3.6) and (3.7), when $n = 0$, i.e the 1-block 3 point method as given in equation (4.1). Thus produces simultaneously values for $y_1 y_2 y_3$, without recourse to any predictor (Lambert 1973) to provide y_1 *and* y_2 in the main method, hence this is an improvement over other reported works. Though, this does not becloud the contribution of these authors.

4.0 Stability Analysis

Recall that, it is a desirable property for a numerical integrator to produce solution that behave similar to the theoretical solution to a problem at all times. Thus several definitions, which call for the method to possess some "adequate" region of absolute stability, can be found in several literatures. See Lambert (1973), Fatunla (1992; 1994) etc. following Fatunla (1992), the three integrator proposed in this paper as stated in equations (3.6) and (3.7) are put in the matrix-equation form and for easy analysis the result was normalized to obtain;

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} y_{n+1} \\ y_{n+2} \\ y_{n+3} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} y_{n-2} \\ y_{n-1} \\ y_n \end{pmatrix} + h$$

$$\left[\begin{pmatrix} \frac{23}{12} & -\frac{4}{3} & \frac{5}{12} \\ \frac{7}{3} & -\frac{2}{3} & \frac{1}{4} \\ \frac{9}{4} & 0 & \frac{3}{4} \end{pmatrix}\begin{pmatrix} f_{n+1} \\ f_{n+2} \\ f_{n+3} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} f_{n-2} \\ f_{n-1} \\ f_{n} \end{pmatrix}\right] \quad (4.1)$$

The first characteristic polynomial of the proposed 1-block 3-point method is

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

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

(4.2)

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

$$= \left\lfloor R^{2}(R-1)\right\rfloor$$

$P(R) = R^2(R-1)$. This implies, $R_1 = R_2 = 0$ or $R_3 = 1$

From definition (1.3) and equation (4.2), the 1 block 3-point is zero stable and is also consistent as its order $(3,3,3)^T > 1$, thus, it is convergent, see Henrici (1962).

Remarks 4.1

Using the matlab package, we were able to plot the stability region of the proposed block method. This is done by reformulating the, 1- block3-point method as general linear method to obtain the values of the matrices A,B,U,V which a re t hen s ubstituted i nto s tability m atrix a nd s tability function. Then the utilized maple package yield the stability polynomial of the block method. T he program yielded t he plot of absolute stability region of the proposed three step block backward differentiation formulae (BDF). From definition (1.1) and figure (4.1) below the proposed three point block (BDF) method (3.6; 3.7) is A − stable.

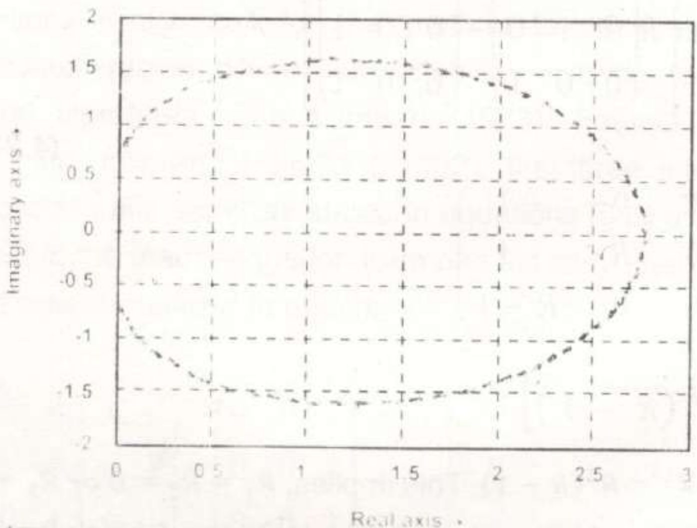

Figure 4.1: Region of Absolute Stability

5.0 NUMERICAL EXPERIMENT

To illustrate the potentials of the new formulas constructed in this paper, we will solve stiff initial value problem while the proposed three points block (BDF) type method is self starting on its own.

Consider the initial value problem

$y' = -10y, \qquad y(2) = 2.06115E-09$

$2 \le x \le 5 \qquad h = 0.2$

$exact \quad solution \quad : \quad y(x) = e^{-10x}$

Table 5.1 proposed (BDF) block method

N	x	Exact value	Approx value	Error
1	2.0	2.0611500E-09	2.0611500E-09	0
2	2.2	2.7894700E-10	4.3926150E-10	1.6031450E-10
3	2.4	3.7751300E-11	3.3789344E-11	3.9619556E-12
4	2.6	5.1090900E-12	3.3789344E-11	2.8680254E-11
5	2.8	6.9144000E-13	7.2010078E-12	6.5095678E-12
6	3.0	9.3576200E-14	5.5392368E-13	4.6034748E-13
7	3.2	1.2664200E-14	5.5392368E-13	5.4125948E-13
8	3.4	1.7139100E-15	1.1804931E-13	1.1633540E-13
9	3.6	2.3195200E-16	9.0807160E-15	8.8487640E-15
10	3.8	3.1391300E-17	9.0807160E-15	9.0493247E-15
11	4.0	4.2483500E-18	1.9352346E-15	1.9309862E-15
12	4.2	5.7495200E-19	1.4886420E-16	1.4828924E-16
13	4.4	7.7811300E-20	1.4886420E-16	1.4878639E-16
14	4.6	1.0530600E-20	3.1725157E-17	3.1714626E-17
15	4.8	1.4251600E-21	2.4403967E-18	2.4389715E-18
16	5.0	1.9287500E-22	2.4403967E-18	2.4402038E-18

Conclusion

We have converted to continuous form the well known 3-step BDF. The continuous formulae are immediately employed as block method for direct solution of first order ivps. The direct solutions are in discrete form which can be substituted into the continuous formula for dense output. The proposed method is self starting, convergent and A – stable as shown by the plotted region of absolute stability (Figure 4.1). The method has been tested on simple ODEs and shown to perform satisfactorly, without recourse to any other method to provide a starting value.

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