A Three-Step Numerical Approximant Based on Block Hybrid Backward Differentiation Formula for Stiff System of Ordinary Differential Equations

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***Abstract* — As long as the field of Engineering, Science and Technology exists, the place of Mathematical modelling that involves stiff systems cannot be overemphasized. Models involving stiff system may result in ordinary differential equations (ODEs) or sometimes as system of ordinary differential equations which must be solved by experts working in that field.However, solving these models using analytical approach may sometimes be challenging or even near impossible. Therefore, it puts a great measure of importance on research into numerical algorithmsfor solution of this class of ordinary differential equations.Premised on the above mentioned, we have formulated, in this paper, a class of backward differentiation formula (BDF) which is a three-step numerical approximant for stiff systems of ODEs. The method was obtained through continuous collocation approach with Legendre polynomial as basis function. We incorporated three off-grid points at interpolation in order that we may retain theBDF's single function evaluation characteristic. Analyzing basic properties of numerical methods led us to see that the method was consistent, having a uniform order six, zero-stable and in turn, convergent. The method's region of absolute stability was determined using the general linear method, which was plotted and shown to be stable over a vast area. The approach enumerates the solution of stiff of systems ODEs block by block using some discrete schemes that are secured from the corresponding continuous scheme. The method was tested using numerical experiments, and the results, when compared to exact or analytical answers as well as some methods published in the literature, proved that the method is efficient and accurate.**

***Keywords* — Ordinary Differential Equations, Stiff system, Backward Differentiation Formula, Hybrid Block method.**

I. INTRODUCTION

At a point where the rate of formation of free radicals in a complex concatenation of events was encountered, with free radicals created and destroyed so swiftly in comparison to the time scale for the overall process, [1] unfolded a method named Backward Differentiation formula, which they adopted in approximating a system of ordinary differential equation,

$$y' = Ay, \quad A \in R^{n\times n}, \tag{1}$$

having a sweeping stiffness ratio. That is,

$$\mathrm{Re}(\lambda_i < 0) \text{ and } q = \frac{\max\{\mathrm{Re}(\lambda_i), i = 1,2,3,...,n\}}{\min\{\mathrm{Re}(\lambda_i), i = 1,2,3,...,n\}} \gg 1.$$

Sometimes, where $q = 10$, the system is thought out to be weakly stiff and stiff if q exceeds 10. Stiff systems are identified by the presence of short-livedand stable components. This peculiarity makes the numerical solution wobbly unless the step size is made abysmal. Owing to this curtailment placed on the choice of step size, numerical solution of stiff system has imposed a great deal of intereston researchers, most of who offered various formulations. In theirsubmissions, [2] and [3] posited that the results given by explicit methods are "consistently unsatisfactory" and "don't do a very good job" respectively. The duoadvocated implicit multistep methods for approximating the problem. Reference [3] even recommended that where possible, one should change one's formulation of problem to avoid solving stiff ordinary differential equation.

Myriads of other researchers have left no stone unturned in ensuring that more implicit methods are provided in solving stiff system of ordinary differential equations. The likes of [4] –[10].

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Reference [1] propounded Backward Differentiation Formula in order that solution of differential equation considered to be stiff,owing to thecurtailmentthat *A-stability* puts on the choice of appropriate methods for stiff systems, several well-heeled efforts have been made by various researchers [5] and [11]-[14], in formulating various BDF based methods, including its higher by-products, for its approximation.

Acategory of linear multi-step methods (LMM) in which off-step points are infused in the derivation process is called hybrid method. It this method, features of linear multi-step methods as well as Runge-Kutta methods are preserved, allowing the Dahlquist Barrier theorem to be beaten. (The order of LMM cannot be more than $k+1$ for k odd or $k+2$ for k even). A *k*-step continuous hybrid according to [5] is of the type

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_k f_{n+j} + h \sum_{j=0}^{k} \beta_v f_{n+v}, \tag{2}$$

where k is the step size,$\alpha_k = 1$, $\alpha_j = 0, 1, \ldots, k-1$ and β_j, are unknown constants.This will be determined in a one-of-a-kind manner. Hybrid approaches are distinguished by their excellent accuracy and broad stability domain.

To solve stiff systems of ordinary differential equations, we formulated a three-step hybrid block backward differentiation formula in this paper.

II. Derivation of the Method

We'll assume that a polynomial of the form

$$y(x) = h \sum_{j=0}^{i+c-1} \alpha_k p_j(x), \tag{3}$$

can approximate the analytical solution of (1), where i and c are respectively, number of interpolation and collocation points,α_j's are coefficients to be determined and $p_j(x)$ can be any orthogonal polynomial. In this situation, the Legendre polynomial is used, which provides exactly the same continuous form as the commonly used power series on inspection.

We included k off-grid sites for each k-step process, which necessitates the fulfillment of the following requirements:

$$y(x_n) = y_n, \tag{4}$$

$$y(x_{n+j}) = y_{n+j},\ j = 0, \left(\frac{1}{2}\right), 1, \ldots k - \frac{1}{2}, \tag{5}$$

$$f(x_{n+k}) = f_{n+k}, \tag{6}$$

where f implies the derivative of y. (4), (5) and (6) result in $(i + c)$ system of equations.The matrix inversion approach is used to solve the system of equations. This is in order to obtain values for j such that the method's

$$y(x) = h \sum_{j=0}^{k-\frac{1}{2}} \alpha_k(x) y_{n+j} + h\beta_k(x) f_k. \tag{7}$$

We set $k = 3,\ i = 5,\ c = 1$ and $x \in [x_n, x_{n+3}]$, which resulted in the system of equation

$$Y_\omega = D\Psi_{\omega-n}, \tag{8}$$

where

$$Y_\omega = \left(y_n, y_{n+\frac{1}{2}}, y_{n+1}, y_{n+\frac{3}{2}}, y_{n+2}, y_{n+\frac{5}{2}}, f_{n+3} \right)^T, \quad \Psi_{\omega-n} = \left(\alpha_0, \alpha_{\frac{1}{2}}, \alpha_1, \alpha_{\frac{3}{2}}, \alpha_2, \alpha_{\frac{5}{2}}, \beta_3 \right)^T \tag{9}$$

and D is a 7×7 matrix. With the help of Maple software and the matrix inversion technique,the values of α_o, $\alpha_{1/2}\, \alpha_1 \alpha_{3/2}$, $\alpha_{2,} \alpha_{5/2}$ and β_3 were obtained, substituted into (7). Setting $k = x - x_n$. The main technique in (10) was obtained by evaluating at $x = x_n + 3h$

$$y_{n+3} = -\frac{10}{147}y_n + \frac{72}{147}y_{n+\frac{1}{2}} - \frac{225}{147}y_{n+1} + \frac{400}{147}y_{n+\frac{3}{2}} - \frac{450}{147}y_{n+2} + \frac{360}{147}y_{n+\frac{5}{2}} + \frac{30}{147}hf_{n+3}. \quad (10)$$

The first derivative of (7) was obtained and evaluated at $x = x_n + 1/2h,\ x = x_n + h,\ x = x_n + 3/2h,\ x = x_n + 2h$ and $x = x_n + 5/2$ hyielding three additional discrete schemes given in (11) to (12). (15).

$$4410hf_{n+\frac{5}{2}} = 300hf_{n+3} - 394y_n + 2925y_{n+\frac{1}{2}} - 9600y_{n+1} + 18700y_{n+\frac{3}{2}} - 26550y_{n+2} + 14919y_{n+\frac{5}{2}} \quad (11)$$

$$-4410hf_{n+2} = 60hf_{n+3} - 167y_n + 1320y_{n+\frac{1}{2}} - 4860y_{n+1} + 12560y_{n+\frac{3}{2}} - 6045y_{n+2} - 2808y_{n+\frac{5}{2}} \quad (12)$$

$$4410hf_{n+\frac{3}{2}} = 30hf_{n+3} - 157y_n + 1395y_{n+\frac{1}{2}} - 6840y_{n+1} + 400y_{n+\frac{3}{2}} + 6165y_{n+2} - 963y_{n+\frac{5}{2}} \quad (13)$$

$$-2205hf_{n+1} = 15hf_{n+3} - 152y_n + 1800y_{n+\frac{1}{2}} + 2460y_{n+1} + -5680y_{n+\frac{3}{2}} + 1980y_{n+2} - 408y_{n+\frac{5}{2}} \quad (14)$$

$$882hf_{n+\frac{1}{2}} = 12hf_{n+3} - 298y_n - 2235y_{n+\frac{1}{2}} + 4320y_{n+1} - 2780y_{n+\frac{3}{2}} + 1290y_{n+2} - 297y_{n+\frac{5}{2}} \quad (15)$$

III. Analysis of the Method

This section examines the fundamental properties of numerical approaches.

A. Order of Accuracy and Error Constant

Following in the footsteps of [15], let $y\left(x_{n+j}\right)$, the solution to $y'\left(x_{n+j}\right)$ be sufficiently differentiable, then $y\left(x_{n+j}\right)$ and $y'\left(x_{n+j}\right)$ can be expanded into a Taylor's series about point x_n to obtain

$$T_n = \frac{1}{h\sigma(1)}\left[C_0 y(x_n) + C_1 hy'(x_n) + C_2 hy''(x_n) + C_1 h^2 y''(x_n) + \dots\right], \quad (16)$$

where

$$C_0 = \sum_{j=0}^{k}\alpha_j,\ C_1 = \sum_{j=0}^{k} j\alpha_j - \sum_{j=0}^{k}\beta_j, \dots,\ C_q = \frac{1}{q!}\sum_{j=0}^{k} j^q\alpha_j - \frac{1}{(q-1)!}\sum_{j=0}^{k} j^{q-1}\beta_j. \quad (17)$$

Definition: A Linear multistep method is said to be of order of accuracy p if $C_0 = C_1 = \dots = C_p = 0$, $C_{p+1} \neq 0$, C_{p+1} is called the error constants.

From our calculations, we have that the block method has uniform order six with error constant

$$C = \begin{pmatrix} -\frac{159}{448} & -\frac{81}{224} & -\frac{501}{896} & -\frac{177}{224} & -\frac{1035}{448} & -\frac{15}{224} \end{pmatrix}^T.$$

B. Consistency

A linear multistep method is said to be consistent if the following conditions are satisfied to the order of accuracy $p > 1$,

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

ii. $\rho'(1) = \sigma(1)$ where $\rho(r)$ and $\sigma(r)$ are respectively, first and second characteristic polynomials of the methods.

Conditions (i) and (ii) were taken care of in section 3.1 since the order $p > 1$ and $C_0 = \sum_{j=0}^{k}\alpha_j = 0$ in all cases. For the third condition, the first and second characteristic polynomials are obtained and evaluated in what follows.For all the methods, conditions for consistency are satisfied. Hence, they are consistent with uniform order of accuracy, $p = 2k > 0$.

C. Zero Stability

The derived Hybrid Backward Differentiation Formula can be written in a block form as follows.

$$A^{(1)}Y_{\omega+1} = A^{(0)}Y_{\omega-1} + hBF_{\omega+1} \tag{18}$$

whose first characteristics polynomial is given as

$$\rho(R) = \det\left[RA^{(1)} - A^{(1)}\right] \tag{19}$$

Definition: The block method (18) is said to be zero stable if no rootof the first characteristic polynomial $\rho(R)$ satisfies $|R_j| \le 1,\ j = 1,2,3,...$ and for those roots with $|R_j| = 1$, the multiplicity must not exceed 2. Expressing methods (10), (11), (12), (13), (14) and (15) in the form (19), we have that

$$\rho(R) = -\frac{134481277728}{12243162971}R^5(R-1) = 0 \text{ and } R = \{0,0,0,0,0,1\}.$$

The method is zero stable having satisfied $|R_j| \le 1$.

D. Convergence

The convergence of the proposed hybrid backward differentiation formula is in accordance with Dahlquist's fundamental theorem, which states, "The necessary and sufficient proviso for a linear multistep procedure to be convergent is for it to be consistent and zero stable" (1962).

The methods created are convergent if they satisfy the necessary and sufficient provisos of consistency and zero stability, according to this theorem.

E. Region of Absolute Stability of the Method

The set $S = \{z \in C : |R_j| \le 1$ is the stability domain, also known as the stability region, of a numerical method. The general linear method (GLM), which is a generalization of Runge-Kutta (multistage) methods and linear multistep (multi-value) methods, was used to find the region of absolute stability.

The derived methods are written in the form

$$\begin{pmatrix} Y \\ y_{i+1} \end{pmatrix} = \begin{pmatrix} A & U \\ B & V \end{pmatrix}\begin{pmatrix} hf(Y) \\ y_{i-1} \end{pmatrix}, \tag{20}$$

Where

$$A = \begin{pmatrix} a_{11} & . & . & . & a_{16} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ a_{16} & . & . & . & a_{66} \end{pmatrix}, B = \begin{pmatrix} b_{11} & . & . & . & b_{16} \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \\ b_{16} & . & . & . & b_{66} \end{pmatrix}, \ Y = \begin{pmatrix} y_n \\ . \\ . \\ . \\ y_{n+3} \end{pmatrix} \text{and } Y_{n+1} = \begin{pmatrix} y_{n+k} \\ . \\ . \\ . \\ y_{n+k-1} \end{pmatrix}.$$

Definition: For a general linear method (A, B, U, V), stability matrix $M(z)$ is defined by

$$M(Z) = V + zB(I - zA)^{-1}U, \tag{21}$$

and the characteristic polynomial is given by

$$\varphi(\mu, z) = \det\left[\mu I - M(z)\right]. \tag{22}$$

Definition: A general linear method (A, B, U, V), is said to be A-stable if for all $z \in C^-$, $I - zA$ is non-singular and $M(z)$ is the stability polynomial.

Definition: A general linear method (A, B, U, V), is said to be L-stable if it is A-stable and $\rho(M(\infty)) = 0$ or the stronger condition, $M(\infty) = 0$.

To obtain and plot region of absolute stability (also known as domain of absolute stability), elements of the matrices A, B, U and V were obtained from interpolation and collocation points and then substituted into the stability matrix (21) and the stability function (22).The stability polynomial is given as

$$\varphi(\mu,z)=\frac{1}{15(164+147z)(-49+10z)(-403+294z)}\begin{pmatrix}6842700\mu^3z^3-33418980\mu^3z^2-1810425\mu^3z-104155380\mu^2z^2+48577620\mu^3\\+55362552\mu^2z+184760416\mu^2+116249805\mu z-105294648\mu-7872300\end{pmatrix}. \qquad (23)$$

The plot of region of absolute stability is shown in Fig. 1 where it is found that the method has a moderate region of absolute stability.

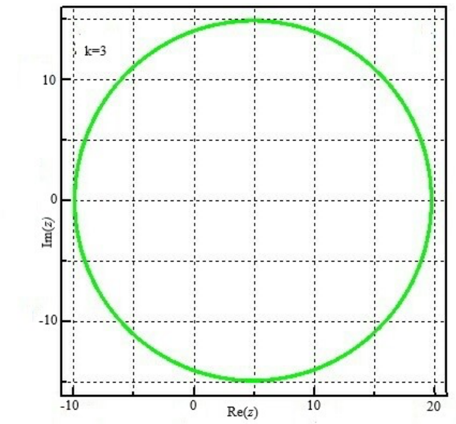

Fig. 1. Region of absolute stability of the method.

The region of absolute stability is the space outside the green boundary.

F. Numerical Experiment

The effectiveness of the suggested strategy is evaluated in this section using a stiff system of ordinary differential equations. By combining the methods as a simultaneous numerical integrator for IVPs, the self-starting method is efficiently achieved.

(1) $y'=-y+95z$, $y(0)=1$, $z'=-y-97z$, $z(0)=1$, $t\in[0,1]$, $h=0.0625,\ 0.03125$.

Exact solution: $y(t)=\frac{95}{47}e^{-2t}-\frac{48}{47}e^{-96t}$, $z(t)=\frac{48}{47}e^{-96t}-\frac{1}{47}e^{-t}$.

This problem was solved in [4], [14] and [16].The absolute error at $t=1$ was obtained and compared as shown in Table I. It is seen that the method performs better than existing methods.

TABLE I: COMPARING THE ABSOLUTE ERROR IN THE PROPOSED METHOD WITH EXISTING METHODS OR PROBLEM 1

h	Reference [17]	Reference [4]	Reference [13]	New Method
	y_n	y_n	y_n	y_n
	z_n	z_n	z_n	z_n
	3.20×10^{-10}	5.00×10^{-8}	3.40×10^{-9}	1.45×10^{-9}
0.06	2.40×10^{-10}	7.00×10^{-10}	3.60×10^{-9}	1.52×10^{-11}
	1.20×10^{-10}	6.00×10^{-8}	3.40×10^{-9}	2.30×10^{-11}
0.03	8.10×10^{-10}	1.00×10^{-10}	3.50×10^{-9}	2.43×10^{-13}

(2) $y_1'=-1002y_1+1000y_2^2$, $y_1(0)=1$, $y_2'=y_1-y_2(1+y_2)$, $y_2(0)=1$

Exact solution: $y_1(x)=e^{-2x}$, $y_2(x)=e^{-x}$, $x\in[0,1]$, $h=0.02$.

This is a non-linear stiff problem solved in [11].We compare the absolute error at $x=1$ with the error obtained in [11] for $h=0.02$ and the proposed method is seen to perform better as shown in Table II.

TABLE II: COMPARING THE ABSOLUTE ERROR IN THE PROPOSED METHOD WITH EXISTING METHODS FOR PROBLEM 2

h	Reference [11]	New Method
	y_{50}	y_{50}
	z_{50}	z_{50}
	9.11×10^{-13}	2.12×10^{-21}
0.02	1.25×10^{-12}	7.89×10^{-17}

IV. Conclusion

Here we have anotherconfiguration of BDF for the approximation of stiff systems of ordinary differential equations is now available. It has a uniform order of 2k, is zero stable, and convergent. The method's efficacy and accuracy were demonstrated by comparing the method's results to those acquired using other methods.

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