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A NEW NUMERICAL INTEGRATOR FOR THE SOLUTION OF STIFF FIRST ORDER ORDINARY DIFFERENTIAL EQUATIONS

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Abstract. This paper considered one step numerical integrator for the solution of first order initial value problems.The method of interpolation of the power series approximate solution and collocation of the differential system to generate a continuous linear multistep method which was evaluated at some selected grid points and implemented in block method was considered.The basic properties of the resultant discrete block method was investigated and found to be zero-stable, consistent and convergent.The numerical integrator was tested on some numerical examples, the results were presented in tabular form and adequately discussed.

Keywords: interpolation, grid points, zero stable, convergent, block method.

2000 AMS Subject Classification: 65L05, 65L06, 65D30

1. Introduction

This paper considered the numerical solution to stiff problem of the form

$$y' = f(x, y.), \quad y(x_0) = y_0, \tag{1.1}$$

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where x_0 is the initial point, y_0 is the solutionat the initial point and f is assumed to be continuous and satisfies the lipschitz theorem for the existence and uniqueness of solution. Most of the physical problems modelled in kenitics, chemical reactions, process control and electrical circuit theory often result to stiff ordinary differential equations (ODEs) where processes with widely varying time constants are usually encountered. It should be recalled that stiff initial value problems were first encountered in the study of motion of spring of varying stiffness, from which the problem derives it name [5].

Definition 1.1 [6] The initial value problem (1.1) is considered to be stiff oscillatory if the eigenvalues $\{\lambda_j = u_j + iv_j,\ j = 1(1)\ m\}$ of the Jacobian $J = \frac{\partial f}{\partial y}$ possess the following properties $u_j < 0,\ j = 1(1)m$,

$$Max 1 \leq j \leq m \left|u_j\right| > Max i \leq j \leq m \left|u_j\right|$$

or if the stiffness ratio satisfies $S = Max i, j \left|\frac{u_i}{u_j}\right| > 1$ and $\left|u_j\right| \ < \left|u_j\right|$ for at least pair of j in $1 \leq j \leq m$.

Most of the conventional numerical solver cannot efficiently cope with stiff problems because they lack the stability characteristics [5]. Most of the methods proposed for the solution of stiff problems are numerically unstable unless the step size are taken to be extremely small. Scholars have reported that the adoption of an implicit schemes which are A-stable method are better for the solution of stiff problems [9].

Definition 1.2 [8] A numerical method is said to be A-stable if the whole of the left-half plane $\{z : Re(z) \leq 0\}$ is contained in the region $\{z : |Re(z) \leq 1|\}$, where $R(z)$ is called the stability polynomial of the method.

scholars have proposed different numerical method for the solution of (1.1) by adopting different approximate polynomial ranging from backward differentiation formula, power series polynomial, fourier series polynomial, Langrange polynomial to mention few. Though, the choice of the approximate solution depends largely on the type of problem to be solved, not withstanding, most of these methods do not give good stability properties hence they fail when the problems is stiff or oscillatory. the introduction of off step method has help greatly in the solution of stiff problem because most of these problems give better stability condition and have circumvented the Dalquist stability barrier [14].

Scholars have proposed different method of implementation ranging from predictor-corrector method to block method. Block method has been reported in literature to be better than the predictor-corrector method in terms of cost of development, time of execution and accuracy was proposed to take care of some of the set backs of the predictor-corrector method; see [1-3], [11-14] and the references therein.

In quest for the method that gives better stability condition, scholars proposed an approximate solution which combined power series polynomial and exponential function [7]. It was discovered that this method gives an A-stable method no matter how the grid points are selected. Still in our quest for method that gives better stability condition. In this paper, we consider the unique properties of hybrid method which is implemeted in block method using the approximate method proposed by [7].

2. Methodology

2.1. Development of the method

We consider a combination of power series and exponential function approximate solution of the form

$$y(x) = \sum_{j=0}^{r+s-2} a_j x^j + a_{r+s-1} e^{\alpha x}, \tag{2.1}$$

where r and s are the numbers of interpolation and collocation points respectively. x^j is the polynomial basis function, $a_j^{\prime} s \in \Re$ are constants to be determined.

Substituting the first derivative of (2.1) into (1.1) yields

$$f(x,y) = \sum_{j=1}^{r+s-2} j a_j x^{j-1} + \alpha a_{r+s-1} e^{\alpha x}. \tag{2.2}$$

Collocating (2.2) at x_{n+r} $r = 0(\frac{1}{4})1$ and interpolating (2.1) at x_{n+s} $s = 0$ gives a system of non -linear equation of the form

$$AX = U, \tag{2.3}$$

where

$$A = [a_0, a_1, a_2, a_3, a_4]^T$$

$$U = [y_n, y_{n+\frac{1}{4}}, y_{n+\frac{2}{4}}, y_{n+\frac{3}{4}}, y_{n+1}]^T$$

and

$$X = \begin{bmatrix} 1 & x_n & x_n^2 & x_n^3 & x_n^4 & (1+\alpha x_n + \frac{\alpha^2 x_n^2}{2!} + \frac{\alpha^3 x_n^3}{3!} \frac{\alpha^4 x_n^4}{4!} \frac{\alpha^5 x_n^5}{5!}) \\ 0 & 1 & 2x_n & 3x_n^2 & 4x_n^3 & (\alpha + \alpha^2 x_n + \frac{\alpha^3 x_n^2}{2!} + \frac{\alpha^4 x_n^3}{3!} \frac{\alpha^5 x_n^4}{4!}) \\ 0 & 1 & 2x_{n+\frac{1}{4}} & 3x_{n+\frac{1}{4}}^2 & 4x_{n+\frac{1}{4}}^3 & (\alpha + \alpha^2 x_{n+\frac{1}{4}} + \frac{\alpha^3 x_{n+\frac{1}{4}}^2}{2!} + \frac{\alpha^4 x_{n+\frac{1}{4}}^3}{3!} \frac{\alpha^5 x_{n+\frac{1}{4}}^4}{4!}) \\ 0 & 1 & 2x_{n+\frac{1}{2}} & 3x_{n+\frac{1}{2}}^2 & 4x_{n+\frac{1}{2}}^3 & (\alpha + \alpha^2 x_{n+\frac{1}{2}} + \frac{\alpha^3 x_{n+\frac{1}{2}}^2}{2!} + \frac{\alpha^4 x_{n+\frac{1}{2}}^3}{3!} \frac{\alpha^5 x_{n+\frac{1}{2}}^4}{4!}) \\ 0 & 1 & 2x_{n+\frac{3}{4}} & 3x_{n+\frac{3}{4}}^2 & 4x_{n+\frac{3}{4}}^3 & (\alpha + \alpha^2 x_{n+\frac{3}{4}} + \frac{\alpha^3 x_{n+\frac{3}{4}}^2}{2!} + \frac{\alpha^4 x_{n+\frac{3}{4}}^3}{3!} \frac{\alpha^5 x_{n+\frac{3}{4}}^4}{4!}) \\ 0 & 1 & 2x_{n+1} & 3x_{n+1}^2 & 4x_{n+1}^3 & (\alpha + \alpha^2 x_{n+1} + \frac{\alpha^3 x_{n+1}^2}{2!} + \frac{\alpha^4 x_{n+1}^3}{3!} \frac{\alpha^5 x_{n+1}^4}{4!}) \end{bmatrix}$$

Solving (2.3) for $a_j's, j = 0(\frac{1}{4})1$ using Gussian elimination method and substituting into (2.1) gives a continuous block method in the form

$$y(x) = \sum_{j=0}^{1} \frac{(jh)^m}{m!} y_n^{(m)} + h\left(\sum_{j=0}^{1} \beta_j(x) f_{n+j} + \beta_k f_{n+k}\right),\ k = \frac{1}{4}, \frac{1}{2}, \frac{3}{4}, \tag{2.4}$$

where

$$\alpha_0 = 1,$$

$$\beta_0 = \frac{8}{45}\left(12t^5 - \frac{75}{2}t^4 + \frac{175}{4}t^3 - \frac{375}{16}t^2 + \frac{45}{8}t\right),$$

$$\beta_{\frac{1}{4}} = -\frac{32}{45}\left(12t^5 - \frac{135}{4}t^4 + \frac{65}{2}t^3 - \frac{45}{4}t\right),$$

$$\beta_{\frac{1}{2}} = \frac{16}{15}\left(12t^5 - 30t^4 + \frac{95}{4}t^3 - \frac{45}{8}t\right),$$

$$\beta_{\frac{3}{4}} = -\frac{32}{45}\left(12t^5 - \frac{105}{4}t^4 + \frac{35}{2}t^3 - \frac{15}{4}t\right),$$

$$\beta_1 = \frac{8}{45}\left(12t^5 - \frac{45}{2}t^4 + \frac{55}{4}t^3 - \frac{45}{16}t\right),$$

$$t = \frac{x - x_n}{h}.$$

Evaluating (2.4) at $t = \frac{1}{4}(\frac{1}{2})1$ gives the discrete block formulae of the form

$$A^{(0)}Y_m = ey_n + h\left[df(y_n) + bf(Y_m)\right], \tag{2.5}$$

where

$$Y_m = \begin{bmatrix} y_{n+\frac{1}{4}} & y_{n+\frac{1}{2}} & y_{n+\frac{3}{4}} & y_{n+1} \end{bmatrix}^T,$$

$$F(Y_m) = \begin{bmatrix} f_{n+\frac{1}{4}} & f_{n+\frac{1}{2}} & f_{n+\frac{3}{4}} & f_{n+1} \end{bmatrix}^T,$$
$$y_n = \begin{bmatrix} y_{n-1} & y_{n-2} & y_{n-3} & y_n \end{bmatrix}^T,$$
$$f(y_n) = \begin{bmatrix} f_{n-1} & f_{n-2} & f_{n-3} & f_n \end{bmatrix}^T.$$

$A^{(0)} = 4 \times 4$ identity matrix

$$e = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$d = \begin{bmatrix} 0 & 0 & 0 & \frac{251}{2880} \\ 0 & 0 & 0 & \frac{29}{360} \\ 0 & 0 & 0 & \frac{27}{320} \\ 0 & 0 & 0 & \frac{7}{90} \end{bmatrix}, \qquad b = \begin{bmatrix} \frac{323}{1440} & -\frac{11}{120} & \frac{53}{1440} & -\frac{19}{2880} \\ \frac{31}{90} & \frac{1}{15} & \frac{1}{90} & -\frac{1}{360} \\ \frac{51}{160} & \frac{9}{40} & \frac{21}{160} & -\frac{3}{320} \\ \frac{16}{45} & \frac{2}{15} & \frac{16}{45} & \frac{7}{90} \end{bmatrix}.$$

2.2. Implementation of the method

In order to implement the method, we propose a prediction equation of the form

$$Y_m^{(0)} = ey_n + h\sum_{\lambda=0}^{3} \frac{\partial^\lambda}{\partial x^\lambda} f(x,y)_{(x_0,y_0)}. \tag{2.6}$$

Substituting (2.6) into (2.4) gives

$$A^{(0)}Y_m = ey_n + h\left[df(y_n) + bdF(Y_m)\right]. \tag{2.7}$$

Hence, (2.7) is our new method.

3. Analysis of Basic Properties of the Method

3.1. Order of the block

Let the linear operator $\mathfrak{L}\{y(x):h\}$ associated with the discrete block method (2.7) be defined as

$$\mathfrak{L}\{y(x):h\} = A^{(0)}Y_m - ey_n - h\left[df(y_n) + bF(Y_m)\right]. \tag{2.8}$$

Expanding (2.7) in Taylor series and comparing the coefficient of h gives

$$\mathfrak{L}\{y(x):h\} = C_0 y(x) + C_1 y^1(x) + \ldots + C_p h^p y^p(x) + C_{p+1} h^{p+1} y^{p+1}(x) + \ldots.$$

Definition 3.1.1. The linear operator $\mathfrak{L}$ and associated block formular are said to be of order p if $C_0 = C_1 = \ldots C_p = C_{p+1} = 0, C_{p+1} \neq 0$. C_{p+1} is called the error constant and implies that the truncation error is given by $t_{n+k} = C_{p+1} h^{p+1} y^{p+1}(x) + 0(h^{p+2})$. For our proposed method, expanding (2.6) in Taylor series and comparing the coefficient of h gives

$$C_7 = \begin{bmatrix} \frac{3}{655360} & \frac{1}{368640} & \frac{3}{655360} & 0 \end{bmatrix}^T.$$

3.2. Zero stability of the method

Definition 3.2.1. A block method is said to be zero stable if as $h \to 0$, the roots, $r_j = 1(1)k$ of the first characteristics polynomials $p(x) = 0$ that is $p(r) = \det\left[\sum A^{(0)} R^{k-1}\right] = 0$ satisfying $|R| \leq 1$ must have multiplicity equal to unity.

For our method

$$p(R) = \left[R \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \right] = 0$$

$p(R) = R^3(R-1) = 0 \Rightarrow R_1 = R_2 = R_3 = 0, R_4 = 1$. Hence, the new block integration is zero-stable.

3.3. Consistency

The block integrator (7) is consistent since it has order $p = 5 \geq 1$.

3.4. Convergence

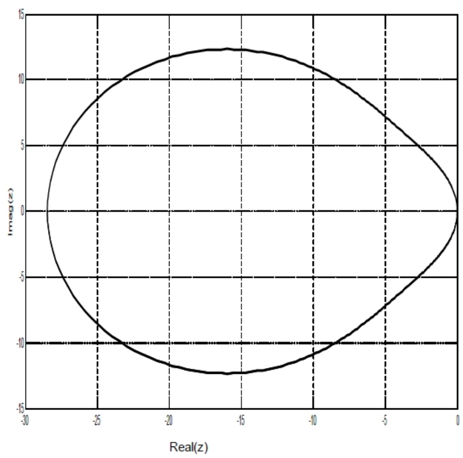
The new block intergator is convergent by the convergence of Dahlquist theorem given below.

Theorem 3.4.1. *The necessary and sufficient conditions that a continuous linear multistep method be convergentare that it must be consistent and zero-stable.*

Definition 3.4.2. Region of absolute stability is a region in the complex $Z-$plane, where $\tau = \lambda h$. τ is defined as those values of Z such that the numerical solution of $y' = -\lambda y$ satisfies $y_j \to 0$ as $j \to \infty$ for any initial value condition.

We adopted the boundary locus method to determine the stability of our method. Substituting $y' = -\lambda h$ into (2.6) gives the stability region as shown in fig 1.

fig. 1. showing stability region of the method



4. Numerical Experiments

In this section, the concern is the application of the schemes derived in section two in block form on some initial value problems with test problems 4.1.1-4.1.3.

4.1. Numerical examples

Problem 4.1.1: $y' = -10(y-1)^2$, $y(0) = 2$, $y(x) = 1 + \frac{1}{(1+10x)}$, $h = 0.01, 0 \leq x \leq 1$.
[source: [9]]

Problem 4.1.2: $y' = xy$, $y(0) = 1$, $y(x) = e^{\frac{x^2}{2}}$, $h = 0.1, 0 \leq x \leq 1$.
[source: [4]]

Problem 4.1.3: $y' = -100xy^2$, $y(1) = \frac{1}{51}$, $y(x) = \frac{1}{(1+50x^2)}$, $h = \frac{1}{4}, \frac{1}{8}, \frac{1}{16}, 0 \leq x \leq 20$.
[source [13] and [10]]

Table 1 Showing results for Problem 4.1.1

X	Error in [9]	Error in NR
0.01	$1.07(-03)$	$5.527220(-005)$
0.02	$2.38(-03)$	$7.520349(-005)$
0.03	$2.21(-03)$	$7.990705(-005)$
0.04	$5.36(-03)$	$7.803322(-005)$
0.05	$7.53(-03)$	$7.346380(-005)$
0.06	$9.00(-03)$	$6.798272(-005)$
0.07	$9.98(-03)$	$6.241065(-005)$
0.08	$1.06(-02)$	$5.711225(-005)$
0.09	$1.10(-02)$	$5.223270(-005)$
0.10	$1.12(-02)$	$4.781142(-005)$

Table 2: Showing results for Problem 4.1.2

X	Err in [3]	Err in NR
0.10	$5.29(-007)$	$2.606759(-011)$
0.20	$1.77(-007)$	$8.431988(-011)$
0.30	$8.99(-007)$	$1.850877(-010)$
0.40	$3.09(-007)$	$3.479586(-010)$
0.50	$1.91(-006)$	$6.051188(-010)$
0.60	$4.48(-006)$	$1.006964(-009)$
0.70	$1.02(-005)$	$1.630994(-009)$
0.80	$7.74(-005)$	$2.595632(-009)$
0.90	$1.44(-005)$	$4.081569(-009)$
1.00	$2.93(-005)$	$6.364684(-009)$

Table 3:Showing results for Problem 4.1.3

h	X	Error in NR	Error in [13]	Error in [10]
$\frac{1}{16}$	10	$0.199960(-03)$	$0.199(-03)$	$0.199(-03)$
		$1.279930(-13)$	$4.470(-09)$	$1.700(-010)$
$\frac{1}{8}$	10	$0.199960(-03)$	$0.199(-03)$	$0.499(-03)$
		$1.018927(-11)$	$4.515(-08)$	$3.090(-09)$
	20	$0.499975(-04)$	$0.499(-04)$	$0.499(-04)$
		$6.370670(-13)$	$2.938(-09)$	$1.950(-10)$
$\frac{1}{4}$	10	$0.199961(-03)$	$0.199(-03)$	$0.200(-03)$
		$9.956010(-10)$	$8.987(-07)$	$4.937(-08)$
	20	$0.499975(-04)$	$0.499(-04)$	$0.500(-04)$
		$6.224663(-11)$	$5.732(-08)$	$3.107(-09)$

4.2. Discussion of result

Problem 4.1.1 was solved by [9] where a three block backward differenciation formula was proposed. Problem 4.1.2 was solved by [3] where a stiff starting block method of order six was proposed. Problem 4.1.3 was solved by [10]. Table 1-3 shows clearly that our method performed better in term of accuracy than the existing method.The method proposed by [13] and [10] are of order six and four respectively.

5. Conclusion

We have proposed a non self starting continuous block method in this paper. The continuous block method enable us to evaluate a given problem at all the points within the interval of integration without starting the block all over.This property enables us to understand the behaviour of a dynamical system at any given point within the interval of integration. It had been shown from the examples given that the non self starting method gives better approximation than the self starting method.

Conflict of Interests

The authors declare that there is no conflict of interests.

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