

Numerical Strategies for the System of First Order IVPs Using Block Hybrid Extended Trapezoidal Multistep Method of Second Kind for Stiff ODEs

Yohanna Sani Awari

Department of Mathematical Sciences, Taraba State University, Jalingo, Nigeria

Email address:

awari04c@yahoo.com

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Abstract: A Modified Three Step Block Hybrid Extended Trapezoidal Multistep Method of Second Kind (BHETR_{2S}) with two off-grid points, one at interpolation and another at collocation point yielding uniform order six (6, 6, 6, 6, 6)^T for the Numerical Integration of initial value problems of stiff Ordinary Differential Equations was developed. The main method and additional equations were obtained from the same continuous formulation through interpolation and collocation procedures. The stability properties of the method was discussed and from the stability region obtained, the method is suitable for the solution Stiff Ordinary Differential Equations. Three numerical examples were considered to illustrate the efficiency and accuracy.

Keywords: Collocation, A-Stability, Hybrid Method, Initial Value Problem, Stiff Differential Equations

1. Introduction

Consider the stiff initial value problem in the form:

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

on the finite interval $I = [x_0, x_N]$, where

$y : [x_0, x_N] \rightarrow R^m$ and $f : [x_0, x_N] \times R^m \rightarrow R^m$ are continuous. By considering the partition

$$I_j = a + jh, \quad j = 0, \dots, N-1, \quad h = \frac{b-a}{N-1}$$

one can consider the k -step LMM

$$\sum_{j=0}^k \alpha_j y_{n+j} = h \left[\sum_{j=0}^k \beta_j(x) f_{n+j} \right] \tag{2}$$

to approximate the solution of problem (1) over the considered partition. As usual, y_{n+j} and f_{n+j} denote the approximations to $y(x_{n+j})$ and $f(x_{n+j}, y(x_{n+j}))$ respectively.

The initial value problem of stiff differential equations occurs in almost every field of science [see 3, 8, 10, 12 and 15], particularly, in the fields of:

A) Chemical Reactions: A famous chemical reaction is the Oregonator reaction between $HBrO_2$, Br^- , and $Ce(IV)$ described by Field and Noyes in 1984.

B) Reaction-diffusion systems: Problems in which the diffusion is modeled via the Laplace operator may become stiff as they are discretized in space by finite differences or finite elements, well-known example of such systems which appear so often in mathematical biology.

Several further occurrences of stiffness can be found in electrical circuits, mechanics, meteorology, oceanography and vibrations.

Definition 1: If the solution of the system contains components which change at significantly different rates for given changes in the independent variable, then system is said to be stiff [8, 15].

Stiff differential equations are characterized as those whose exact solution has a term of the form $e^{-\lambda t}$, where λ is a large positive constant. The key features of stiff equations are that the derivative terms may increase rapidly as t

increases [12].

In the last three decades numerous works have been focusing on the development of more advanced and efficient methods for stiff problems [8, 12]. The situation becomes more complicated when stiffness coupled with nonlinearity. Carroll presents an exponential fitted scheme for solving stiff systems of initial value problems [15]. The numerical solution of linear and nonlinear system of stiff system can be found in [3, 11 and 12].

Block methods were introduced to both improve the stability of methods and provide the $k - 1$ starting values to $k - step$ LMM. They can be seen as a set of linear multistep methods simultaneously applied to (1) and then combined to yield better approximations (Ajie, et al., 2014).

2. Formulation of the Method

A more elegant and computationally attractive

$$\begin{aligned} \phi_0(x) &= 1 - \frac{1225 \xi}{303 h} + \frac{8035 \xi^2}{1212 h^2} - \frac{3419 \xi^3}{606 h^3} + \frac{3187 \xi^4}{1212 h^4} - \frac{193 \xi^5}{303 h^5} + \frac{19 \xi^6}{303 h^6} \\ \phi_1(x) &= -\frac{22016 \xi^3}{101 h^3} + \frac{17268 \xi^2}{101 h^2} - \frac{3876 \xi^5}{101 h^5} + \frac{13329 \xi^4}{101 h^4} - \frac{5040 \xi}{101 h} + \frac{436 \xi^6}{101 h^6} \\ \phi_2(x) &= -\frac{4017 \xi^5}{101 h^5} + \frac{60687 \xi^2}{404 h^2} - \frac{40631 \xi^3}{202 h^3} + \frac{475 \xi^6}{101 h^6} - \frac{4365 \xi}{101 h} + \frac{52203 \xi^4}{404 h^4} \\ \phi_3(x) &= \frac{29440 \xi}{303 h} - \frac{99328 \xi^2}{303 h^2} + \frac{23872 \xi^5}{303 h^5} - \frac{2752 \xi^6}{303 h^6} + \frac{128704 \xi^3}{303 h^3} - \frac{79936 \xi^4}{303 h^4} \\ \psi_1(x) &= \frac{11947 \xi^4}{303 h^3} - \frac{6953 \xi^3}{101 h^2} + \frac{17704 \xi^2}{303 h} - \frac{1940 \xi}{101} + \frac{364 \xi^6}{303 h^5} - \frac{1112 \xi^5}{101 h^4} \\ \psi_2(x) &= \frac{7359 \xi^4}{202 h^3} - \frac{8167 \xi^2}{202 h} + \frac{5584 \xi^3}{101 h^2} + \frac{1155 \xi}{101} - \frac{142 \xi^6}{101 h^5} + \frac{1166 \xi^5}{101 h^4} \\ \psi_3(x) &= \frac{704 \xi^2}{303 h} - \frac{64 \xi}{101} + \frac{704 \xi^4}{303 h^3} + \frac{32 \xi^6}{303 h^5} - \frac{336 \xi^3}{101 h^2} - \frac{80 \xi^5}{101 h^4} \end{aligned}$$

Evaluating the continuous formulation in (3) yields the $BHETR_2$ associated with the continuous scheme and converting it into A, B, U and V of the General Linear Method (12) as:

0	0	0	0	0	0	0	0	0	1
$-\frac{101}{5040}$	$-\frac{388}{1008}$	0	$\frac{231}{1008}$	$-\frac{4}{315}$	0	$-\frac{97}{112}$	$\frac{5888}{3024}$	0	$-\frac{35}{432}$
0	$-\frac{159}{112}$	$-\frac{303}{56}$	$-\frac{387}{244}$	$\frac{3}{56}$	0	$\frac{4023}{448}$	0	$-\frac{891}{112}$	$-\frac{11}{448}$
0	$-\frac{113}{633}$	0	$\frac{530}{1477}$	$-\frac{256}{4431}$	$\frac{101}{13293}$	0	$\frac{68864}{39879}$	$-\frac{152}{211}$	$-\frac{257}{39879}$
0	$-\frac{75}{404}$	0	$\frac{675}{808}$	$\frac{15}{101}$	0	$-\frac{675}{1616}$	$\frac{225}{101}$	$-\frac{325}{404}$	$-\frac{9}{1616}$
0	$\frac{366}{101}$	0	$-\frac{738}{101}$	$\frac{192}{101}$	0	$\frac{2187}{101}$	$-\frac{3584}{101}$	$\frac{1485}{101}$	$\frac{13}{101}$
0	$\frac{366}{101}$	0	$-\frac{738}{101}$	$\frac{192}{101}$	0	$\frac{2187}{101}$	$-\frac{3584}{101}$	$\frac{1485}{101}$	$\frac{13}{101}$
0	$-\frac{113}{633}$	0	$\frac{530}{1477}$	$-\frac{256}{4431}$	$\frac{101}{13293}$	0	$\frac{68864}{39879}$	$-\frac{152}{211}$	$-\frac{257}{39879}$
0	$-\frac{159}{112}$	$-\frac{303}{56}$	$-\frac{387}{244}$	$\frac{3}{56}$	0	$\frac{4023}{448}$	0	$-\frac{891}{112}$	$-\frac{11}{448}$
$-\frac{101}{5040}$	$-\frac{388}{1008}$	0	$\frac{231}{1008}$	$-\frac{4}{315}$	0	$-\frac{97}{112}$	$\frac{5888}{3024}$	0	$-\frac{35}{432}$

3. Order, Convergence and Absolute Stability Region

3.1. Order of BHETR_{2S}

Definition 2

A linear multistep method (3) is consistent if it has order $p \geq 1$.

According to [9], a LMM is said to be of order p if $c_0 = c_1 = c_2 = \dots = c_p = 0, c_{p+1} \neq 0$, this approach can be

$$\begin{pmatrix} \alpha_{01} & \alpha_{11} & \alpha_{21} & \dots & \alpha_{k1} \\ \alpha_{02} & \alpha_{12} & \alpha_{22} & \dots & \alpha_{k2} \\ \alpha_{03} & \alpha_{13} & \alpha_{23} & \dots & \alpha_{k3} \\ \dots & \dots & \dots & \dots & \dots \\ \alpha_{0k} & \alpha_{1k} & \alpha_{2k} & \dots & \alpha_{kk} \end{pmatrix} \begin{pmatrix} y_n \\ y_{n+1} \\ y_{n+2} \\ \dots \\ y_{n+k} \end{pmatrix} = h \begin{pmatrix} \beta_{01} & \beta_{11} & \beta_{21} & \dots & \beta_{k1} \\ \beta_{02} & \beta_{12} & \beta_{22} & \dots & \beta_{k2} \\ \beta_{03} & \beta_{13} & \beta_{23} & \dots & \beta_{k3} \\ \dots & \dots & \dots & \dots & \dots \\ \beta_{0k} & \beta_{1k} & \beta_{2k} & \dots & \beta_{kk} \end{pmatrix} \begin{pmatrix} f_n \\ f_{n+1} \\ f_{n+2} \\ \dots \\ f_{n+k} \end{pmatrix} \quad (6)$$

The expression (6) is equivalent to (5) where,

$$\bar{\alpha}_0 = \begin{pmatrix} 01 \\ 02 \\ 03 \\ \dots \\ 0k \end{pmatrix}, \bar{\alpha}_1 = \begin{pmatrix} 11 \\ 12 \\ 13 \\ \dots \\ 1k \end{pmatrix}, \dots, \bar{\alpha}_k = \begin{pmatrix} k1 \\ k2 \\ k3 \\ \dots \\ kk \end{pmatrix} \text{ and } \bar{\beta}_0 = \begin{pmatrix} 01 \\ 02 \\ \dots \\ 0k \end{pmatrix},$$

$$\bar{\beta}_1 = \begin{pmatrix} 11 \\ 12 \\ 13 \\ \dots \\ 1k \end{pmatrix}, \dots, \bar{\beta}_k = \begin{pmatrix} k1 \\ k2 \\ k3 \\ \dots \\ kk \end{pmatrix} \quad (7)$$

Adopting the order procedure used in the single case for the block method and recall that

$$L_h y(x) = \sum_{i=0}^k [\bar{\alpha}_i y(x+ih) - h \bar{\beta}_i f(x+ih, y(x+ih))] \quad (8)$$

where, $y(x)$ is the exact solution satisfying (1). Carrying out

extended to determine the order of the entire block method which can be expressed as:

$$\sum_{i=0}^k \alpha_{ij} y_{n+j} = h \sum_{i=0}^k \beta_{ij} f_{n+j} \quad (5)$$

where, $j = 0, 1, \dots, k$ is a positive integer, equation (5) can be expanded to give the following system of equation

Taylor series expansion on (8) about x yields the equation

$$L_h y(x) = \bar{c}_0 y(x) + \bar{c}_1 h y'(x) + \bar{c}_2 h^2 y''(x) + \dots + \bar{c}_p h^p y^{(p)}(x) \quad (9)$$

$$\bar{c}_0 = \begin{pmatrix} c_{01} \\ c_{02} \\ c_{03} \\ \dots \\ c_{0p} \end{pmatrix}, \bar{c}_1 = \begin{pmatrix} c_{11} \\ c_{12} \\ c_{13} \\ \dots \\ c_{1p} \end{pmatrix}, \dots, \bar{c}_p = \begin{pmatrix} c_{p1} \\ c_{p2} \\ c_{p3} \\ \dots \\ c_{pp} \end{pmatrix} \quad (10)$$

From (4), the coefficients of (7) are obtained as

$$\bar{\alpha}_0 = \left(-\frac{13}{101}, \frac{9}{1616}, \frac{257}{303}, -\frac{11}{2424}, \frac{1225}{303}, 0 \right)^T$$

$$\bar{\alpha}_1 = \left(-\frac{1485}{101}, \frac{325}{404}, \frac{9576}{101}, -\frac{297}{202}, \frac{5040}{101}, 0 \right)^T$$

$$\bar{\alpha}_2 = \left(\frac{3584}{101}, \frac{225}{101}, -\frac{68864}{303}, -\frac{56}{303}, -\frac{29440}{303}, 0 \right)^T$$

$$\bar{\alpha}_3 = \left(-\frac{2187}{101}, \frac{675}{1616}, \frac{13293}{101}, \frac{1341}{303}, \frac{4365}{101}, 0 \right)^T$$

$$\bar{\alpha}_3 = (1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 0)^T$$

$$\bar{\alpha}_2^s = (0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0)^T$$

and

$$\bar{\beta}_0 = (0 \quad 0 \quad 0 \quad 0 \quad -1 \quad 0)^T$$

$$\bar{\beta}_1 = \left(\frac{366}{101} \quad -\frac{150}{808} \quad -\frac{2373}{101} \quad \frac{106}{404} \quad -1 \quad 0 \right)^T$$

$$\bar{\beta}_2 = (0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0)^T$$

$$\bar{\beta}_3 = \left(-\frac{738}{101} \quad \frac{675}{808} \quad \frac{4770}{101} \quad \frac{129}{404} \quad \frac{1155}{101} \quad 0 \right)^T$$

$$\bar{\beta}_4 = (0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0)^T$$

$$\bar{\beta}_5 = \left(\frac{192}{101} \quad \frac{120}{808} \quad -\frac{768}{101} \quad -\frac{4}{404} \quad -\frac{64}{101} \quad 0 \right)^T$$

Applying (8)-(10), yields a uniformly sixth order for the BHETR_{2s}, which is presented in table (1).

Definition 3A-Stability[4]

A numerical method (4) 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 4

The method presented in (4) is said to be of order p if

$c_0 = c_1 = c_2 = \dots = c_p$ and $c_{p+1} \neq 0$, c_{p+1} is called the error constant and the local truncation error given by

$$T_n = \bar{c}_{p+1} h^{p+1} y^{(p+1)}(x_n) \tag{11}$$

3.2. Absolute Stability Region

To determined the absolute stability region of the block method, they are reformulated into General Linear Methods of [2] where they used as partition $(s+r)(s+r)$ matrix containing A, B, U and V expressed as (4) in the form

$$\begin{bmatrix} Y \\ y^{i-1} \end{bmatrix} = \begin{bmatrix} A & U \\ B & V \end{bmatrix} \begin{bmatrix} hf(Y) \\ y^i \end{bmatrix}, i = 1, 2, \dots, N \tag{12}$$

Where the matrices A, B, U and V are substituted into a stability matrix

$$M(z) = V + zB(I - zA)^{-1}U \tag{13}$$

Which is in-turn substituted into a stability function

$$\rho(\lambda, z) = \det(\lambda I - Mz) \tag{14}$$

The values of A, U, B, V in (7) are substituted in (5) to obtain the stability matrix. Plotting the stability matrix in MATLAB code to obtain the region of absolute stability of the block hybrid method as shown in Figure 1.

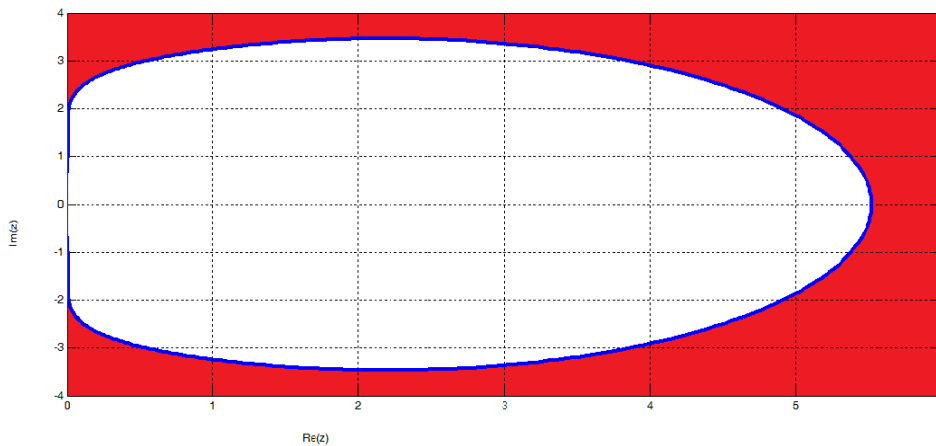


Figure 1. Region of absolute stability of the block hybrid method.

Note:

- a. Figure 1 presents the region of absolute stability of the block hybrid method and is shown to be the entire shaded portion including the left hand half complex plane (in agreement with definition 3)
- a. Analysis from the graph (Figure 1) suggests that the block hybrid method proposed in this paper would be suitable to solve stiff ordinary differential equations.

3.3. Convergence

Following [5], the BHETR_{2s} (4) can be represented by a matrix finite difference equation in the form:

$$A^{(0)} y_{m+1} = \sum_{i=1}^k A^{(i)} y_{m+1} + h \sum_{i=0}^k B^{(i)} f_{m-1} \tag{15}$$

where

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

$$B_1 = \begin{bmatrix} \frac{673}{360} & -\frac{104}{45} & \frac{211}{120} & -\frac{32}{45} & \frac{43}{360} \\ \frac{1323}{640} & -\frac{77}{40} & \frac{1053}{640} & -\frac{27}{40} & \frac{73}{640} \\ \frac{92}{45} & -\frac{224}{135} & \frac{29}{15} & -\frac{32}{45} & \frac{16}{135} \\ \frac{2375}{1152} & -\frac{125}{72} & \frac{875}{384} & -\frac{35}{72} & \frac{125}{1152} \\ \frac{81}{40} & -\frac{8}{5} & \frac{81}{40} & 0 & \frac{11}{40} \end{bmatrix} \text{ and}$$

$$B_0 = \begin{bmatrix} 0 & 0 & 0 & 0 & \frac{11}{40} \\ 0 & 0 & 0 & 0 & \frac{35}{128} \\ 0 & 0 & 0 & 0 & \frac{37}{135} \\ 0 & 0 & 0 & 0 & \frac{35}{128} \\ 0 & 0 & 0 & 0 & \frac{11}{40} \end{bmatrix}$$

Definition 5: A block method is zero stable provided the roots $\lambda_j = 1, 2, \dots, k$ of the first characteristic polynomial $\rho(\lambda)$ specified as

$$\rho(\lambda) = \det \left[\sum_{i=0}^k A^{(i)} \lambda^{k-i} \right] = 0 \tag{16}$$

satisfies $|\lambda_j| \leq 1$, the multiplicity must not exceed two, [6]

Following (16), we have that

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

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

$$\rho(\lambda) = \lambda^4(\lambda - 1) = 0$$

Thus, $\lambda_1 = 1, \lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = 0$. By definition 5, the BHETR_{2S} method is zero stable.

4. Implementation Strategies

In this section, we have tested the performance of our three-step block method on three (3) numerical Initial Value Problems of first order ODEs. For each example; we find the absolute errors of the approximate solution.

Example 4.1: We consider the Initial Value Problem with step-size $h = 0.1$

$$\frac{dy}{dx} - xy = 0, y(0) = 1$$

Analytical Solution of the given problem is $y(x) = e^{\frac{x^2}{2}}$

Table 1. Maximum Errors for Example 4.1.

X	Maximum Error in[13]	Maximum Error in the New Block Hybrid Method
0.1	5.29E-007	3.165E-009
0.2	1.77E-007	3.172E-009
0.3	8.99E-007	3.439E-009
0.4	3.09E-007	1.625E-008
0.5	1.91E-006	1.683E-008
0.6	4.48E-006	1.843E-008
0.7	1.02E-005	5.456E-008
0.8	7.74E-005	5.833E-008
0.9	1.44E-005	6.522E-008
1.0	2.93E-005	1.668E-007

Example 4.2: The SIR model is an epidemiological model that computes the theoretical numbers of people infected with a contagious illness in a closed population over time. The name of this class of models derives from the fact that they involves coupled equations relating the number of

susceptible people $S(t)$, number of people infected $I(t)$ and the number of people who have recovered $R(t)$. This is a good and simple model for many infectious diseases including measles, mumps and rubella [13-15]. The SIR

model is described by the three coupled equations.

$$\frac{ds}{dt} = \mu(1 - S) - \beta IS$$

$$\frac{dI}{dt} = -\mu I - \gamma I + \beta IS$$

$$\frac{ds}{dt} = -\mu R + \gamma I$$

where μ, γ and β are positive parameters. Define y to be $y = S + I + R$

Adding all these equations give

$$y' = \mu(1 - y)$$

Taking $\mu = 0.5$ and attaching an initial condition $y(0) = 0.5$ (for a particular closed population), we obtain

$$y'(t) = 0.5(1 - y), y(0) = 0.5$$

Whose analytical solution is $y(t) = 1 - 0.5e^{-0.5t}$

Table 2. Maximum Errors for Example 4.2.

X	Analytical Solution	Numerical Solution for the New Block Hybrid Method	Maximum Error in [18]	Maximum Error in the New Block Hybrid Method
0.1	0.524385287749643	0.524385287750215	5.574430E-012	5.72E-013
0.2	0.547581290982020	0.547581290982560	3.946177E-012	5.40E-013
0.3	0.569646011787471	0.569646011787959	8.183232E-012	4.88E-013
0.4	0.590634623461009	0.590634623461945	3.436118E-011	9.36E-013
0.5	0.610599608464298	0.610599608465186	1.929743E-010	8.88E-013
0.6	0.629590889659141	0.629590889659952	1.879040E-010	8.11E-013
0.7	0.647655955140644	0.647655955141798	1.776835E-010	1.154E-012
0.8	0.664839976982180	0.664839976983277	1.724676E-010	1.097E-012
0.9	0.681185924189114	0.681185924190118	1.847545E-010	1.004E-012
1.0	0.696734670143684	0.696734670144944	3.005770E-010	1.260E-012

Example 4.3: Consider the test problem $\frac{dy}{dx} - \lambda y = 0, y(0) = 1$, with solution $y = e^{\lambda x}$ is solved with $h = 0.01$ and $\lambda = -5$.

Table 3. Maximum Errors for Example 4.3.

X	Analytical Solution	Numerical Solution for the New Block Hybrid Method	Maximum Error in [1] Order 7	Maximum Error in the New Block Hybrid Method Order 6
0.02	0.904837418035960	0.904837418034642	8.57E-012	1.318E-012
0.04	0.818730753077982	0.818730753075408	7.79E-012	2.574E-012
0.06	0.740818220681718	0.740818220679243	7.00E-012	2.475E-012
0.08	0.670320046035639	0.670320046032424	1.33E-011	3.215E-012
0.10	0.606530659712633	0.606530659708700	1.18E-011	3.933E-012
1.12	0.548811636094026	0.548811636090359	1.07E-011	3.667E-012

Table 4. Order and Error Constants of the Method.

Method	Order p	Error Constants
4	6	$\frac{71}{56560}$
	6	$\frac{15}{361984}$
	6	$\frac{243}{28280}$
	6	$\frac{29}{1357440}$
	6	$\frac{107}{33936}$
	6	$\frac{107}{33936}$

5. Conclusions

We have developed a modified three-step block hybrid extended trapezoidal multistep method of second kind with two off-grid points, yielding uniform order six (table 4) for the numerical integration of initial value problems of stiff

ordinary differential equations. The new block methods are self- starting and all the discrete schemes used were obtained from the single continuous formulation and its derivative which are of uniform order of accuracy. Implementation of our method in block form tends to speed up computational process. Results obtained from our method shows significant improvement when compared with results of existing

authors. Our sixth order block hybrid method performs better than the seventh order method of Ajie *et al.*, (see table 3).

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