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A New Multi-Step Approach based on Top Order Methods (TOMs) for the Numerical Integration of Stiff Ordinary Differential Equations

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Abstract

This paper presents an entirely new approach to obtaining self-starting Top Order Methods (TOMs) which we shall called Extended Top Order Methods (ETOMs). ETOMs were obtained through hermite polynomial used as basis function. Stability analysis of the new approach shows a uniform order six method for k = 3, they also possess very good absolute stability regions which made them highly suitable for the numerical integration of stiff ordinary differential equations. Implementation of the method in block form eliminates the need for starters and hence, generating simultaneously approximate solutions y_i, i = 1, 2, ..., 6on the go. To further observe the effect of the new approach, it was implemented on four numerical initial value problems of stiff ordinary differential equations occurring in real life and was shown to compete favorably with the work of existing scientists.

Keywords: Trapezoidal Method, Hermite Polynomial, Top Order Methods, Stiff Equation, Block Method, Stiff ODEs.

1. Introduction

Many field of applications, notably Science and Technology yields initial value problems of first order ordinary differential equations. Some of these equations may not be easily solved theoretically, therefore numerical methods are provided as a means to approximating their solutions. A potentially good numerical method for the solution of stiff system of ODEs of the form

$$y' = f(t, y),\ y'(t_0) = y_0, t \in [t_0, T_n] \tag{1}$$

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must have good accuracy and some reasonably wide region of absolute stability [5, 12]. One of the first and most important stability requirements particularly for linear multistep method is A-stability which was proposed in [6, 12]. However, the requirement of A-stability put some limitations on the choice of suitable LMMs.

Top Order Method (TOM) is group into a family of Boundary Value Methods (BVMs) and was introduced by [3]. According to these authors, the method belongs to the group of symmetric Schemes.

Boundary Value Methods have also been extensively discussed by the following authors: [4, 7, 8].

A. ***Symmetric schemes***

Brugnano grouped as symmetric schemes BVMs having the following general properties:

a. They have an odd number of steps, $k = 2v - 1,\ v \geq 1,$ and must be used with $(v, v-1)$ –boundary conditions (that is, they require $v-1$ initial and $v-1$ final additional methods).

b. The corresponding polynomials $\rho(z)$ have skew-symmetric coefficients. That is

$$z^k \rho(z^{-1}) = -\rho(z);$$

c. The corresponding polynomials $\sigma(z)$ have symmetric coefficients. That is

$$z^k \sigma(z^{-1}) = \sigma(z)$$

d. $D_{v,v-1} \equiv \subset^{-}$

B. **Lemma**: *The sixth order Top Order Method is symmetric*.

Proof:

From the first discrete scheme, we get that

$$\alpha_3 = \frac{11}{60},\ \alpha_2 = \frac{27}{60},\ \alpha_1 = -\frac{27}{60},\ \alpha_0 = -\frac{11}{60} \text{ and } \beta_3 = \frac{1}{20},\ \beta_2 = \frac{9}{20},\ \beta_1 = \frac{9}{20},\ \beta_0 = \frac{1}{20}$$

i. Consider the LHS of (b) in subsection A , we obtained

$$\rho(z^{-1}) = \frac{11}{60}z^{-3} + \frac{27}{60}z^{-2} - \frac{27}{60}z^{-1} - \frac{11}{60}$$

Then,

$$z^3\rho(z^{-1}) = \frac{11}{60} + \frac{27}{60}z^1 - \frac{27}{60}z^2 - \frac{11}{60}z^3$$

Now, RHS of (b), yields

$$-\rho(z) = -\frac{11}{60}z^3 - \frac{27}{60}z^2 + \frac{27}{60}z^1 + \frac{11}{60}$$

ii. From the LHS of (c), we have that

$$\sigma(z^{-1}) = \frac{1}{20}z^{-3} + \frac{9}{20}z^{-2} + \frac{9}{20}z^{-1} + \frac{1}{20}$$

$$z^3\sigma(z^{-1}) = z^3\left[\frac{1}{20}z^{-3} + \frac{9}{20}z^{-2} + \frac{9}{20}z^{-1} + \frac{1}{20}\right]$$

$$= \frac{1}{20} + \frac{9}{20}z^1 + \frac{9}{20}z^2 + \frac{1}{20}z^3$$

From RHS of (c), yields

$$\sigma(z) = \frac{1}{20}z^3 + \frac{9}{20}z^2 + \frac{9}{20}z^1 + \frac{1}{20}$$. In both cases, RHS=LHS. QED

So far, scholars are finding it difficult to derive schemes from the same continuous formulation in form of TOMs that can effectively be implemented in block form for the approximate solution of first order ordinary differential equations of the form (1).

The approach by [3], yields self starting block TOMs however, with some boundary conditions provided, called initial additional equation(s) and final additional equations. The equations were obtained from three or more different formulae.

The author [1], constructed block methods by pairing k -step Top Order Methods (TOMs) with $2k$ -step Backward Differentiation Formulas (BDF) and then shifting the equations $2k-2$ times.

The approach which has been adopted in this paper allows for flexibility of obtaining all the discrete schemes from the same continuous formulation of the main method and then implementing in block form, thereby eliminating the need for starters and pairing. The boundary condition imposed by some referred scholars (that is, the $v-1$ initial and $v-1$ final additional equations stated above) is also eliminated.

2. Derivation of the Method

The approach adopted in this paper entails substituting into (1) a trail solution of the form

$$y(x) = \sum_{j=0}^{s+r-1} a_j H^j(x) \tag{2}$$

where s and r are the interpolation and collocation points, $H^j(x)$ is the hermite polynomial generated by the formula:

$$H_n = (-1)^n e^{\left(\frac{x^2}{2}\right)} \frac{d^n}{dx^n} e^{\left(-\frac{x^2}{2}\right)} \tag{3}$$

For sake of reporting, we present some few terms of the hermite polynomial as

$H_0(x)=1$, $H_1(x)=x$, $H_2(x)=x^2-1$, $H_3(x)=x^3-3x$, $H_4(x)=x^4-6x^2+3$, $H_5(x)=x^5-10x^3+15x$, $H_6(x)=x^6-15x^4+45x^2-15$

From (2)

$$y'(x) = \sum_{j=0}^{s+r-1} j a_j H^{j-1}(x) \tag{4}$$

putting (4) into (1) we obtained

$$f(x,y) = \sum_{j=0}^{s+r-1} j a_j H^{j-1}(x) \tag{5}$$

Interpolating (2) at $x_i, i=1$ and collocating (5) at $x_i, i=0,1,\ldots,3$ gives a system of equation which can be put in the form

$$M_1 z_1 = u_1 \tag{6}$$

where,

$$M_1 = \begin{bmatrix} 1 & 0 & -1 & 0 & 3 & 0 & -15 \\ 1 & h & (h^2-1) & (h^3-3h) & (h^4-6h^2+3) & (h^5-10h^3+15h) & (h^6-15h^4+45h^2-15) \\ 1 & 2h & (12h^2-3) & (8h^3-6h) & (16h^4-24h^2+3) & (32h^5-80h^3+30h) & (64h^6-240h^4+180h^2-15) \\ 0 & 1 & 0 & -3 & 0 & 15 & 0 \\ 0 & 1 & 2h & (3h^2-3) & (4h^3-12h) & (5h^4-30h^2+15) & (6h^5-60h^3+90h) \\ 0 & 1 & 4h & (12h^2-3) & (32h^3-24h) & (80h^4-120h^2+15) & (192h^5-480h^3+180h) \\ 0 & 1 & 6h & (27h^2-3) & (108h^3-36h) & (405h^4-270h^2+15) & (1458h^5-1620h^3+270h) \end{bmatrix}$$

$z_1 = [a_0 \quad a_1 \quad a_2 \quad a_3 \quad a_4 \quad a_5 \quad a_6]^T$ and

$u_1 = [y_n \quad y_{n+1} \quad y_{n+2} \quad hf_n \quad hf_{n+1} \quad hf_{n+2} \quad hf_{n+3}]^T$

Solving (6) for the $a_j,\ j = 0,1,\ldots,6$ yields

$$a_0 = -\frac{27}{4}\frac{\psi^2}{h^2} + \frac{45}{4}\frac{\psi^3}{h^3} - \frac{15}{2}\frac{\psi^4}{h^4} + 1 + \frac{9}{4}\frac{\psi^5}{h^5} - \frac{1}{4}\frac{\psi^6}{h^6}$$

$$a_1 = \frac{36}{11}\frac{\psi^2}{h^2} + \frac{12}{11}\frac{\psi^5}{h^5} - \frac{15}{11}\frac{\psi^4}{h^4} - \frac{20}{11}\frac{\psi^3}{h^3} - \frac{2}{11}\frac{\psi^6}{h^6}$$

$$a_2 = -\frac{147}{44}\frac{\psi^5}{h^5} - \frac{415}{44}\frac{\psi^3}{h^3} + \frac{153}{44}\frac{\psi^2}{h^2} + \frac{19}{44}\frac{\psi^6}{h^6} + \frac{195}{22}\frac{\psi^4}{h^4}$$

$$a_3 = -\frac{82}{33}\frac{\psi^4}{h^3} + \frac{183}{44}\frac{\psi^3}{h^2} - \frac{5}{66}\frac{\psi^6}{h^5} - \frac{109}{33}\frac{\psi^2}{h} + \frac{31}{44}\frac{\psi^5}{h^4}$$

$$a_4 = -\frac{467}{44}\frac{\psi^4}{h^3} + \frac{145}{11}\frac{\psi^3}{h^2} - \frac{19}{44}\frac{\psi^6}{h^5} - \frac{63}{11}\frac{\psi^2}{h} + \frac{79}{22}\frac{\psi^5}{h^4}$$

$$a_5 = -\frac{37}{11}\frac{\psi^4}{h^3} + \frac{151}{44}\frac{\psi^3}{h^2} - \frac{2}{11}\frac{\psi^6}{h^5} - \frac{27}{22}\frac{\psi^2}{h} + \frac{59}{44}\frac{\psi^5}{h^4}$$

$$a_6 = \frac{13}{132}\frac{\psi^4}{h^3} - \frac{1}{11}\frac{\psi^3}{h^2} + \frac{1}{132}\frac{\psi^6}{h^5} + \frac{1}{33}\frac{\psi^2}{h} - \frac{1}{22}\frac{\psi^5}{h^4} \qquad (7)$$

substituting (7) into (2) for $s = 3$ and $r = 4$ gives

$$\begin{aligned}
y(x) = & \left(-\frac{27}{4}\frac{\xi^2}{h^2} + \frac{45}{4}\frac{\xi^3}{h^3} - \frac{15}{2}\frac{\xi^4}{h^4} + 1 + \frac{9}{4}\frac{\xi^5}{h^5} - \frac{1}{4}\frac{\xi^6}{h^6} \right) y_n \\
& + \left(\frac{36}{11}\frac{\xi^2}{h^2} + \frac{12}{11}\frac{\xi^5}{h^5} - \frac{15}{11}\frac{\xi^4}{h^4} - \frac{20}{11}\frac{\xi^3}{h^3} - \frac{2}{11}\frac{\xi^6}{h^6} \right) y_{n+1} \\
& + \left(-\frac{147}{44}\frac{\xi^5}{h^5} - \frac{415}{44}\frac{\xi^3}{h^3} + \frac{153}{44}\frac{\xi^2}{h^2} + \frac{19}{44}\frac{\xi^6}{h^6} \right. \\
& \qquad \left. + \frac{195}{22}\frac{\xi^4}{h^4} \right) y_{n+2} \\
& + \left(\xi - \frac{82}{33}\frac{\xi^4}{h^3} + \frac{183}{44}\frac{\xi^3}{h^2} - \frac{5}{66}\frac{\xi^6}{h^5} - \frac{109}{33}\frac{\xi^2}{h} + \frac{31}{44}\frac{\xi^5}{h^4} \right) f_n \\
& + \left(-\frac{467}{44}\frac{\xi^4}{h^3} + \frac{145}{11}\frac{\xi^3}{h^2} - \frac{19}{44}\frac{\xi^6}{h^5} - \frac{63}{11}\frac{\xi^2}{h} + \frac{79}{22}\frac{\xi^5}{h^4} \right) f_{n+1} \\
& + \left(-\frac{37}{11}\frac{\xi^4}{h^3} + \frac{151}{44}\frac{\xi^3}{h^2} - \frac{2}{11}\frac{\xi^6}{h^5} - \frac{27}{22}\frac{\xi^2}{h} + \frac{59}{44}\frac{\xi^5}{h^4} \right) f_{n+2} \\
& + \left(\frac{13}{132}\frac{\xi^4}{h^3} - \frac{1}{11}\frac{\xi^3}{h^2} + \frac{1}{132}\frac{\xi^6}{h^5} + \frac{1}{33}\frac{\xi^2}{h} - \frac{1}{22}\frac{\xi^5}{h^4} \right) f_{n+3}
\end{aligned} \tag{8}$$

Definition 1: *A numerical method is said to be of order* p *if* $c_0 = c_1 = c_2 = \ldots = c_p$ *and* $c_{p+1} \neq 0$, c_{p+1} *is called the error constant.*

Evaluated (8) at some points of interest yields the desired sixth order Extended Top Order Methods

$$\frac{1}{60}(11y_{n+3} + 27y_{n+2} - 27y_{n+1} - 11y_n) = \frac{h}{20}(f_n + 9f_{n+1} + 9f_{n+2} + f_{n+3})$$

order $p = 6,\ c_p = -\frac{1}{2800}$

$$\frac{1}{600}(281y_{n+3} + 27y_{n+2} - 297y_{n+1} - 11y_n) = \frac{h}{200}(43f_{n+1} + 123f_{n+2} + 35f_{n+3} - f_{n+4})$$

order $p = 6,\ c_p = -\frac{47}{1540}$

$$\frac{1}{42180}(23436y_{n+5}-4725y_{n+4}-18700y_{n+3}-11y_n)=\frac{h}{703}(105f_{n+3}+450f_{n+4}+153f_{n+5}-5f_{n+6})$$

order $p=6,\ c_p=-\frac{345}{77}$

$$\frac{1}{2}(y_{n+3}-y_{n+1})=\frac{h}{180}(-f_n+34f_{n+1}+114f_{n+2}+34f_{n+3}-f_{n+4})$$

order $p=6,\ c_p=\frac{5}{42}$

$$\frac{1}{170}(93y_{n+4}-16y_{n+3}-77y_{n+2})=\frac{h}{15300}(-11f_n+2360f_{n+2}+9800f_{n+3}+3255f_{n+4}-104f_{n+5})$$

order $p=6,\ c_p=\frac{328}{231}$

$$\frac{1}{230}(131y_{n+5}-32y_{n+4}-99y_{n+3})=\frac{h}{62100}(-11f_n+8770f_{n+3}+39825f_{n+4}+13986f_{n+5}-470f_{n+6})$$ order

$p=6,\ c_p=\frac{1191}{154}$

The first equation is shifted $n=n+3$ times and in combination with other discrete schemes; they are perfectly netted together in block form to generate simultaneously the values of $y_i, i=1,2,\ldots,6$ for the numerical solution of (1).

3. Analysis of the Method

C. *Region of absolute stability of the Extended Top Order Methods (ETOMs)*

Solving the characteristics equations of ETOMs, that is $\det(r(A-Cz)-B)=0$ for r, we obtain the stability function in the following ways

$$fz=-\frac{121}{371078550000000}r^5\begin{pmatrix}9268800rz^6-37858920rz^5-645748z^5+16252121z^4+91440260rz^4\\-44157850z^3-146727150rz^3+156087800rz^2-77811740z^2\\-10189800rz-72930600z-30488400+30488400r\end{pmatrix} \tag{9}$$

differentiating (9) to get (10)

$$fzp=-\frac{121}{371078550000000}r^5\begin{pmatrix}55612800rz^5-189294600rz^4-3228740z^4-65008484z^3\\+365761040rz^3-132473550z^2-440181450rz^2+312175600rz\\-155623480z-101089800r-72930600\end{pmatrix} \quad (10)$$

Dividing equation (9) by (10) to obtain the stability function (11)

$$R(z)=\frac{\begin{pmatrix}9268800rz^6-37858920rz^5-645748z^5+16252121z^4+91440260rz^4\\-44157850z^3-146727150rz^3+156087800rz^2-77811740z^2\\-10189800rz-72930600z-30488400+30488400r\end{pmatrix}}{\begin{pmatrix}55612800rz^5-189294600rz^4-3228740z^4-65008484z^3\\+365761040rz^3-132473550z^2-440181450rz^2+312175600rz\\-155623480z-101089800r-72930600\end{pmatrix}} \quad (11)$$

Plotting (11) into MatLab code yields the absolute stability region of the Extended Top Order Methods below

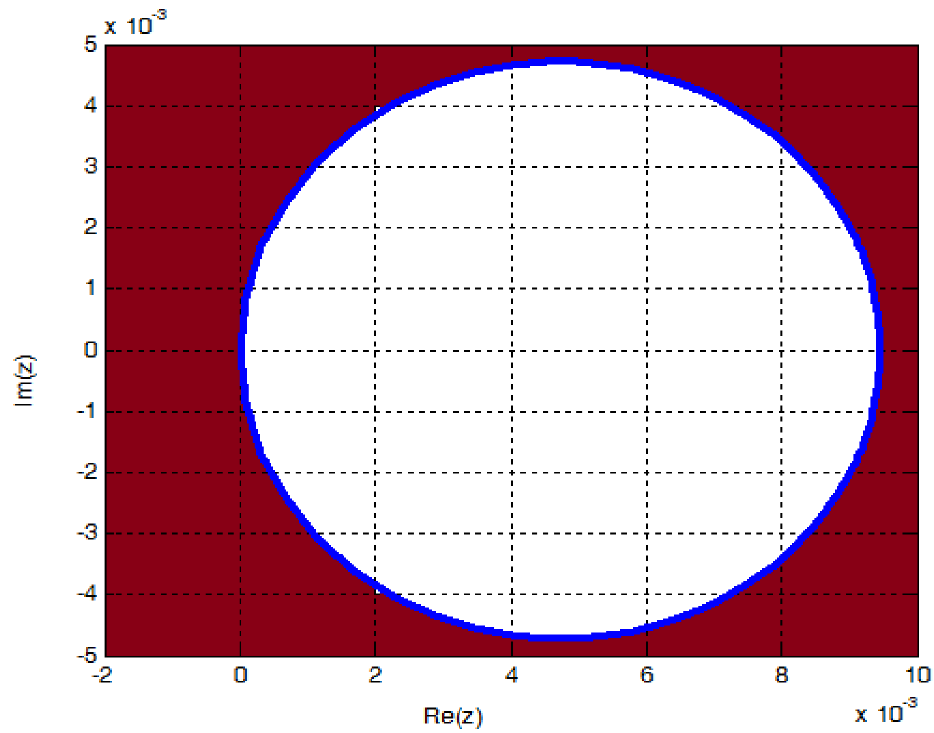

Figure 1: Completely A-Stable ETOMs

Definition 2: *A numerical method is said to be A-stable if its region of absolute stability contains, the whole of the left-hand half plane* $Reh\lambda < 0$

4. Numerical Implementation

Example 4.1: 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 [9-11]. The SIR model is described by the three coupled equations.

$$\frac{ds}{dt} = \mu(1-S) - \beta IS \text{ and } \frac{dI}{dt} = -\mu I - \gamma I + \beta IS \text{ and } \frac{ds}{dt} = -\mu R + \gamma I$$

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 1: Absolute Errors for Example 4.1

X	Error in [14] $p = 6$	Error in ETOMs $p = 6$
0.2	3.946177E-012	2.914E-012
0.4	3.436118E-011	3.48E-012
0.6	1.879040E-010	1.364E-012
0.8	1.724676E-010	9.170E-012
1.0	3.005770E-010	1.577E-012
1.2	-	2.003E-012

1.4	-	2.160E-013
1.6	-	3.570E-013
1.8	-	2.196E-013
2.0	-	7.012E-013

Example 4.2: Consider a highly stiff ordinary differential equation

$$\frac{dy}{dx} - \lambda y = 0 \, , \lambda = -10^6 \, , 0 \le x \le 1 \, , h = 0.1$$

Table 2: Errors for Example 4.2

X	Error in [13] 4^{th} *order method*	Error in [13] 6^{th} *order method*	Error in ETOMs $p = 6$
0.2	2.49×10^{-1}	1.67×10^{-1}	6.54×10^{-2}
0.4	6.24×10^{-2}	3.00×10^{0}	1.54×10^{-3}
0.6	1.56×10^{-2}	5.00×10^{-1}	3.96×10^{-2}
0.8	3.90×10^{-3}	9.00×10^{0}	2.59×10^{-3}
1.0	9.76×10^{-4}	1.50×10^{0}	6.10×10^{-5}
1.2	2.44×10^{-4}	2.70×10^{1}	1.57×10^{-3}
1.4	6.10×10^{-5}	4.50×10^{0}	1.03×10^{-4}
1.6	1.52×10^{-5}	8.10×10^{1}	2.42×10^{-6}
1.8	3.81×10^{-6}	1.35×10^{1}	6.21×10^{-5}
2.0	9.52×10^{-7}	2.43×10^{2}	4.06×10^{-6}

Example 4.3: 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 3: Maximum Errors for Example 4.3

X	Theoretical Solution	Approximate Solution of ETOMs	Error in [9]	Error in ETOMs
0.1	1.00501252085940	1.00501242569890	5.29E-007	9.516E-008
0.2	1.02020134002676	1.02020128492574	1.77E-007	5.510E-008
0.3	1.04602785990872	1.04602775890690	8.99E-007	1.010E-007
0.4	1.08328706767496	1.08328699334416	3.09E-007	7.433E-008
0.5	1.13314845306683	1.13314834060707	1.91E-006	1.125E-007
0.6	1.19721736312181	1.19721734591591	4.48E-006	1.721E-008
0.7	1.27762131320489	1.27762053049684	1.02E-005	7.827E-007
0.8	1.37712776433596	1.37712725489948	7.74E-005	5.094E-007
0.9	1.49930250005677	1.49930158822846	1.44E-005	9.118E-007
1.0	1.64872127070013	1.64872050644375	2.93E-005	7.643E-007

Example 4.4: Consider the discharge valve on a 200-gallon tank that is full of water opened at time $t = 0$ and 3 gallons per second flow out. At the same time 2 gallons per second of 1 percent chlorine mixture begin to enter the tank. Assume that the liquid is being stirred so that the concentration of chlorine is consistent throughout the tank. The task is to determine the concentration of chlorine when the tank is half full. It takes 100 seconds for this moment to occur, since we lose a gallon per second. If $y(t)$ is the amount of chlorine in the tank at time t, then the rate chlorine is entering is $\frac{2}{100}$ gal/sec and it is leaving at the rate $3\left[\frac{y}{200-t}\right]$ gal/sec.

Thus, the resulting IVP is

$$\frac{dy}{dt} = \frac{2}{100} - 3\frac{y}{200-t},\ 0 \le t \le 1,\ y(0) = 0,\ h = 0.1$$

whose analytical solution is

$$y(t) = 2 - \frac{1}{100}t - 2\left[1 - \frac{5t}{1000}\right]^3$$

Source: Areo *et al*., (2013, 2014)

Table 4: Maximum Errors for Example 4.4

X	Theoretical Solution	Approximate Solution of ETOMs	Error in [2] 6th Order Method	Error in ETOMs
0.1	0.00199850025000	0.00199850025000016	0	1.6×10^{-16}
0.2	0.00399400200000	0.00399400200000018	0	1.8×10^{-16}
0.3	0.00598650675000	0.00598650675000016	2.40×10^{-11}	1.6×10^{-16}
0.4	0.00797601600000	0.007976016000000018	2.40×10^{-11}	1.8×10^{-16}
0.5	0.00996253125000	0.00996253125000018	2.40×10^{-11}	1.8×10^{-16}
0.6	0.01194605400000	0.0119460540000002	3×10^{-11}	2.0×10^{-16}
0.7	0.01392658575000	0.0139265857500004	3×10^{-11}	4.0×10^{-16}
0.8	0.01590412800000	0.0159041280000005	3×10^{-11}	5.0×10^{-16}
0.9	0.01787868225000	0.0178786822500003	3×10^{-11}	3.0×10^{-16}
1.0	0.01985025000000	0.0198502500000006	3×10^{-11}	6.0×10^{-16}

5. Conclusion

This paper has been able to derived TOMs (called ETOMs) schemes from the same continuous formulation and was effectively implemented in block form for the numerical approximate of first order ordinary differential equations of the form (1). Stability analysis of the method showed a uniformly order six method for $k = 3$. Figure 1 presents the region of absolute stability of the block ETOMs and was shown to be the entire shaded portion including the left hand half complex plane (fulfilling definition 2). From the graph, the A-stability property of the method was established, making them highly suitable for the numerical integration of stiff ordinary differential equations. Implementation of the method in block form generates simultaneously approximate solutions $y_i, i = 1,2,...,6$ on the go, thereby eliminating the need for starters and pairing. This approach also eliminates the restriction imposed by some scholars (boundary conditions). Table (1-4) shows better performance of the ETOMs in terms of accuracy over existing methods.

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