

A FAMILY OF EXPONENTIALLY FITTED MULTIDERIVATIVE METHOD FOR STIFF DIFFERENTIAL EQUATIONS

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ABSTRACT.

In this paper, an A-stable exponentially fitted predictor-corrector using multiderivative linear multistep method for solving stiff differential equations is developed. The method which is a two-step third derivative method of order five contains free parameters. The numerical stability analysis of the method was discussed, and found to be A-stable. Numerical examples are provided to show the efficiency of the method when compared with existing methods in the literature that have solved the set of problems.

Keywords: Exponentially fitted, Multiderivative linear multistep, stiff differential equations, A-stable.

1.0 INTRODUCTION

In order to solve stiff initial value problems in ordinary differential equations efficiently, many new methods have been developed in recent years, which satisfy certain stability requirements.

The property of A-stability is desirable in formulas to be used in the solution of stiff systems of differential equations especially from chemical kinetics and the discretisation of partial differential equations. Dahlquist [7], proved that A-stable linear multistep formulas must be implicit, its maximum order is two and of those of second order, the one with the smallest truncation error coefficient is the trapezoidal rule. In nearly every linear systems of differential equation, which have widely disperse eignevalues, high order A-stable formulas are particularly appropriate since they allow integration to proceed with a larger step size.

Thus, the need to develop a high order A-stable implicit multistep formula, which uses linear combinations of derivatives higher than the first, give rise to the development of multiderivative multistep formulas. Lambert [11], and Enright [8], pointed out that Multiderivative methods give high accuracy and possess good stability properties when used to solve first order initial value problems in ordinary differential equation.

However, A-stable multiderivative multistep formulas designed for solving stiff systems of differential equations includes, Enright [8], Jackson and Kenue[10], Brown [5], Okunuga[13], Otunta and Abhulimen[15], [3] Abhulimen and Omeike[2].

2.0 THE GENERAL MULTIDERIVATIVE MULTISTEP METHOD

The general multiderivative multistep method is given by,

$$\sum_{i=0}^{k} \alpha_{i} y_{n+i} = \sum_{j=1}^{s} h^{j} \sum_{i=0}^{k} \gamma_{j,i} f_{n+i}^{(j-1)}, \qquad n = 0, 1, 2$$
(2.1)

Where $f_{n+i}^{(j)}$ is the j^{th} derivative of f(x, y) evaluated at (x_{n+1}, y_{n+1}) , α_i and $\gamma_{j,i}$ are real constants with $\alpha_k \neq 0$ and y_{n+1} is the appropriate numerical solution evaluated at the point x_{n+i} . In order to remove the arbitrary constant in (2.1) we shall always assume that $\alpha_k = +1$, and $\sum_{i=0}^k |\alpha_i| > 0$ and $\sum_{i=0}^k |\gamma_{j,i}| > 0$ j = 1, 2, ..., s

2.1 DEVELOPMENT OF NEW EXPONENTIALLY FITTED MULTIDERIVATIVE METHODS

A numerical integration formula is said to be exponentially fitted at (complex) value $\lambda = \lambda_0$ if when the method is applied to the scalar test problem $y' = \lambda h$, $y(x_0) = y_0$, with exact initial condition, the characteristic equation $\phi(\lambda h)$ satisfies the relation $\phi(\lambda_0 h) = e^{\lambda_0 h}$.

However, the idea of using exponentially fitted formulas for the appropriate numerical integration of certain classes of stiff systems of first order ordinary differential equation of the form,

$$y' = f(x, y), \ y(x_0) = y_0$$
 (1.1)

which was originally proposed by Liniger and Willoughby [12], is to derive integration formulas containing free parameters (other than the step length of integration) and then to choose these parameters so that a given function (e^q) , where q is real, satisfies the integration formula exactly.

Liniger and Willoughby [12] derived three 1-step integration formulas with orders ranging from 1 - 3. Their results revealed that for all choices of the fitting parameter q, their formulas are A-stable.



2.2 DERIVATION OF FAMILY OF TWO STEP EXPONENTIALLY FITTED METHODS

The objective of this paper is to develop a two-step, third derivative multiderivative exponentially fitted formulas. (i.e. k = 2 and s = 3).

For this purpose, equation (2.1) is reduced to,

$$\sum_{i=0}^{k} \alpha_{i} y_{n+i} = h \sum_{i=0}^{k} \gamma_{1,i} f_{n+i} + h^{2} \sum_{i=0}^{k} \gamma_{2,i} f_{n+i}^{(1)} + h^{3} \sum_{i=0}^{k} \gamma_{3,i} f_{n+i}^{(2)}$$
(2.2)

Where $\beta_i = \gamma_{1,i}$, $\phi = \gamma_{2,i}$, $\omega_i = \gamma_{3,i}$

From equation (2.2), we obtain

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i} + h^2 \sum_{i=0}^{k} \phi_i g_{n+i} + h^3 \sum_{i=0}^{k} \omega_i v_{n+i}$$
(2.3)

And

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k+1} \beta_i f_{n+i} + h^2 \sum_{i=0}^{k} \phi_i g_{n+i} + h^3 \sum_{i=0}^{k} \omega_i v_{n+i}$$
(2.4)

However, the implementation of the proposed formulas involves a pair of formulas, that is predictor and corrector formulas. Thus, equation (2.3) serves as the predictor and while equation (2.4) serves as the corrector.

where,

$$f_{n+i} = f[x_{n+i}, y(x_{n+i})] = y'_{n+i} \text{and} g_{n+i} = f'[x_{n+i}, y(x_{n+i})] = y''_{n+i}$$
$$v_{n+i} = f''[x_{n+i}, y(x_{n+i})] = y''_{n+i}$$
(2.

are respectively the first, second and third derivatives of y_{n+i} . When we are deriving exponentially fitted multistep methods, the approach is to allow both (2.3) and (2.4) to posses free parameters order than the mesh size '*h*' which allow it to be fitted automatically to exponential function.

2.3 DERIVATION OF METHOD OF FIFTH ORDER FORMULAS

The derivation of predictor-corrector integrations formula of order 5 involves two stages as was done in higher order. First we derived the order four predictor by setting $c_0 = c_1 = c_2 = c_3 = c_4 = 0$ in equation (2.3) to obtain five set of equations with 12 unknown parameters and we then obtain the following set of simultaneous equations

 $a_0 + 1 = 0$ $\beta_0 + a = 2$ $\phi_0 + \phi_2 + 2a = 2$ $6\phi_2 + 6a + 3\omega_0 = 4$ $3\phi_2 + 2a = 1$

When we solve the above equations we obtain,

$$\bar{\alpha}_0 = -1, \bar{\alpha}_2 = 1, \bar{\beta}_0 = 2 - a, \bar{\phi}_0 = \frac{5}{3} - \frac{4}{3}a, \bar{\phi}_2 = \frac{1}{3} - \frac{2}{3}a, \bar{\omega}_0 = \frac{2}{3} - \frac{2}{3}a$$

When these values of the parameters are substituted into (2.3), we obtain the predictor formula as:

$$\bar{y}_{n+2} - \bar{y}_n = h[ay'_{n+2} + (2-a)y'_n] + h^2 \left[\left(\frac{1}{3} - \frac{2}{3}a\right)y''_{n+2} + \left(\frac{5}{3} - \frac{4}{3}a\right)y''_n \right] + h^3 \left[\left(\frac{2}{3} - \frac{2}{3}a\right)y''_n \right]$$
(2.7)

Now, for exponential fitting purpose, we apply (2.7) to scalar test function

 $y' = \lambda y$, y(0) = 1to obtain equation (2.8) below.

$$\frac{\bar{y}_{n+2}}{y_n} = \frac{1 + (2-a)q + \left(\frac{5}{3} - \frac{4}{3}a\right)q^2 + \left(\frac{2}{3} - \frac{2}{3}a\right)q^3}{1 + aq - \left(\frac{1}{3} - \frac{2}{3}a\right)q^2} = R(\bar{q})$$
(2.9)

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(2.6)



For the purpose of stability analysis, we obtain the free parameter a from (2.9).

But from equation ... $\frac{\bar{y}_{n+2}}{y_n} = e^{2q}$ then equation (2.9) yields,

$$a = \frac{1 + 2q + \frac{1}{3}q^2(5 + e^{2q}) + \frac{2}{3}q^3 - e^{2q}}{\frac{2}{3}q^2(2 + e^{2q}) + q(1 + e^{2q}) + \frac{2}{3}q^3}$$
(2.10)

Again to obtain the corresponding order 5 corrector formula, we obtain six set of simultaneous equation from (2.4)asfollows,

$$\alpha_{0} + 1 = 0$$

$$\beta_{0} + b + \beta_{2} = 2$$

$$2\beta_{2} + 3b + \phi_{0} + \phi_{2} = 2$$

$$6\beta_{2} + \frac{27}{2}b + 6\phi_{2} + 3\omega_{0} = 4$$

$$4\beta_{2} + \frac{27}{2}b + 6\phi_{2} = 2$$

$$10\beta_{2} + \frac{405}{8}b + 20\phi_{2} = 4$$

$$(2.11)$$

We impose the same condition as in predictor, and in addition, we let $\beta_3 = b$ as free parameters $\alpha_2 = 1$, the values of the unknown parameters are obtained from (2.11) as,

$$\alpha_0 = -1, \alpha_2 = 1, \beta_0 = \frac{6}{5} - \frac{43}{16}b, \beta_2 = \frac{4}{5} + \frac{27}{16}b, \beta_3 = b$$

$$\phi_0 = \frac{3}{5} - 3b, \phi_2 = -\frac{1}{5} - \frac{27}{8}b, \omega_0 = \frac{2}{15} - \frac{9}{8}b$$

When these values are substitute into (2.4), we obtain the fifth order corrector formula as,

$$y_{n+2} - y_n = h \left[b_3 y'_{n+3} + \left(\frac{4}{5} + \frac{27}{16}b\right) y'_{n+2} + \left(\frac{6}{5} - \frac{43}{16}b\right) y'_n \right] + h^2 \left[\left(-\frac{1}{5} - \frac{27}{8}b\right) y''_{n+2} + \left(\frac{8}{5} + \frac{33}{16}b\right) y''_n \right] + h^3 \left[\left(\frac{2}{15} - \frac{9}{8}b\right) y''_n \right]$$

$$(2.12)$$

By applying (2.12) to test function (2.8) we obtain,

$$\frac{y_{n+2}}{y_n} = \frac{1 + \left(\frac{6}{5} - \frac{43}{16}b\right)q + bq \cdot \frac{y_{n+3}}{y_n} + \left(\frac{8}{5} + \frac{33}{16}b\right)q^2 + \left(\frac{2}{15} - \frac{9}{8}b\right)q^3}{1 - \left(\frac{4}{5} + \frac{27}{16}b\right)q + \left(\frac{1}{5} + \frac{27}{8}b\right)q^2} = R(q)$$
(2.13)

We need to obtain the relation $\frac{y_{n+3}}{y_n}$ in (2.13) for the purpose of exponential fitting condition and stability. From the solution of test function (2.8), we established that;

$$\frac{y_{n+2}}{y_n} = e^{2q} = R(\bar{q})$$
Also, $\frac{y_{n+3}}{y_n} = e^{3q} = (e^{2q})^{\frac{3}{2}}$

$$\frac{\bar{y}_{n+3}}{y_n} = [R(\bar{q})]^{\frac{3}{2}}$$
(2.14)

Equation (2.13) now becomes

$$\frac{y_{n+2}}{y_n} = \frac{1 + \left(\frac{6}{5} - \frac{43}{16}b\right)q + bq \cdot \left[\bar{R}_2(q)\right]^{\frac{3}{2}} + \left(\frac{3}{5} - 3b\right)q^2 + \left(\frac{2}{15} - \frac{9}{8}b\right)q^3}{1 - \left(\frac{4}{5} + \frac{27}{16}b\right)q + \left(\frac{1}{5} + \frac{27}{8}b\right)q^2} = R(q)$$
(2.15)

Equation (2.15) now unites both the parameter and corrector formulas which is capable of solving stiff systems. We obtain the value of the free parameter b from (2.15) as,



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$$b(q) = \frac{1 + \frac{1}{5}(bq + 3q^2) + \frac{2}{15}q^3 + \frac{4}{5}qe^{2q} - e^{2q}\left(1 + \frac{1}{5}q^2\right)}{\frac{27}{8}q^2e^{2q} - 3q^2 + \frac{9}{8}q^3 - \frac{1}{16}(27qe^{2q} - 43q) - qe^{3q}}$$
(2.16)

3.0 STABILITY CONSDIERATION OF THE METHOD

To examine the stability conditions required by this method, it is expected by maximum modulus theorem that the stability function of the method given by (2.16) satisfies |R(q)| < 1.

In order to determine the interval of absolute stability of the method, we find limits of both a(q) and b(q) as $q \to 0$ and $q \to -\infty$

$$\lim_{q \to -\infty} a(q) = \lim_{q \to -\infty} \left[\frac{1 + 2q + \frac{1}{3}q^2(5 + e^{2q}) + \frac{2}{3}q^3 - e^{2q}}{\frac{2}{3}q^2(2 + e^{2q}) + q(1 + e^{2q}) + \frac{2}{3}q^3} \right] = 1$$

$$\lim_{q \to 0} a(q) = \lim_{q \to 0} \left[\frac{1 + 2q + \frac{1}{3}q^2(5 + e^{2q}) + \frac{2}{3}q^3 - e^{2q}}{\frac{2}{3}q^2(2 + e^{2q}) + q(1 + e^{2q}) + \frac{2}{3}q^3} \right] = \frac{4}{5}$$

That is $a \in \left(\frac{4}{5}, 1\right)$ of $q \in (-\infty, 0]$,

Similarly, from (2.16) we have,

$$\lim_{q \to -\infty} b(q) = \lim_{q \to -\infty} \left[\frac{1 + \frac{1}{5}(6q - 8q^2) + \frac{2}{15}q^3 + \frac{4}{5}qe^{2q} - e^{2q}\left(1 + \frac{1}{5}q^2\right)}{\frac{27}{8}q^2e^{2q} - \frac{33}{16}q^2 + \frac{9}{8}q^3 - \frac{1}{16}(27qe^{2q} - 43q) - qe^{3q}} \right] = \frac{16}{135}$$
$$\lim_{q \to 0} b(q) = \lim_{q \to 0} \left[\frac{1 + \frac{1}{5}(6q - 8q^2) + \frac{2}{15}q^3 + \frac{4}{5}qe^{2q} - e^{2q}\left(1 + \frac{1}{5}q^2\right)}{\frac{27}{8}q^2e^{2q} - \frac{33}{16}q^2 + \frac{9}{8}q^3 - \frac{1}{16}(27qe^{2q} - 43q) - qe^{3q}} \right] = \frac{8}{405}$$

Thus we formed that $a \in \left(\frac{4}{5}, 1\right)$ and $b \in \left(\frac{8}{405}, \frac{16}{135}\right)$

Now, we further verify analytically that the ranges of value of *a* and*b* represent the region of absolute stability of the new method. We illustrate this by taking a large sample *S* as shown in table 3.1 below;

q	а	b
-10	0.955214724	0.0989973
-100	0.995050247	0.1163663
-500	0.999002002	0.1180848
-1000	0.999500500	0.1183014
-5000	0.999900020	0.1184751
-10000	0.999950005	0.1184968
-20000	0.999975001	0.11850765

Table 3.1: Parameters values of a and b

From the table above, we observed that as q decreases, the values of a andbare monotonically increasing.

The implication of the observation is that, for any of value of q in the open left-half plane, the corresponding values of a(q) and b(q) converges and bounded within the ranges of $a \in \left(\frac{4}{5}, 1\right)$ and $b \in \left(\frac{8}{405}, \frac{16}{135}\right)$ respectively. These ranges help to determine the region of absolute stability of the new method.

Furthermore, we examine the stability function of the new method. From equation (2.15), the stability function of the new method is given as



$$\tau^* = \frac{1 + \left(\frac{6}{5} - \frac{43}{16}b\right)q + bq \cdot \left[\bar{R}_2(q)\right]^{\frac{3}{2}} + \left(\frac{3}{5} - 3b\right)q^2 + \left(\frac{2}{15} - \frac{9}{8}b\right)q^3}{1 - \left(\frac{4}{5} + \frac{27}{16}b\right)q + \left(\frac{1}{5} + \frac{27}{8}b\right)q^2}$$

When we tested for the values of $q \in (-\infty, 0]$, with the region of absolute stability $a \in (\frac{4}{5}, 1)$ and $b \in (\frac{8}{405}, \frac{16}{135})$, we observed that $|\tau^*(q)| < 1$. Hence, by definition of A-stability of multistep method, we conclude that the new method is A-stable. The new method can solve stiff problems in ordinary differential equations.

4.0 NUMERICAL EXPERIMENTS

In the section, the Numerical Integrators derived are tested on several standard stiff value problems (IVPs) in Ordinary Differential Equations (ODEs).

To show the effectiveness and validity of our newly derived methods, we present some numerical examples below. All numerical examples are coded in Fortan 77 and implemented on digital computer.

However, for purpose of comparative analysis on the performance of the new scheme we denote AL⁵ as the new method, CH4, CH5-Cash [6] method of order 4 and 5 respectively, J-K Jackson and Kenue[10], OK6-Okunuga [13], AB7, AB8, NM9 represent Abhulimen and Otunta[3] method of order 7, 8 and 9 respectively. F⁵ Abhulimen[4] method of order 5, AF5-Abhulimen and Okunuga[1] and AG6-Abhulimen and Omeike[2].

Example 1

Non-linear stiff problems (Enright and Pryce) [9]

$$y'_{1} = -0.013y_{1} + 1000y_{1}y_{3}, y_{1}(0) = 1$$

$$y'_{2} = -2500y_{2}y_{3}, y_{2}(0) = 1$$

$$y'_{3} = 0.013y_{1} - 1020y_{1}y_{3} - 2500y_{2}y_{3}, y_{3}(0) = 0$$
(4.1)

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Step length h	Method	<i>y</i> ₁	$y_2(1)$	$y_{3}(1)$
0.0625	AL⁵	0.5882826881	1.0092403605	-2.7914604750
	AB8	0.5884667145	1.0090563343	-2.7919757498
0.1	AL⁵	0.5882826902	1.0092403584	-2.7914604809
	AB8	0.5882826902	1.0092403584	-2.7914604809
Exact Solution		0.5882826881	1.0092403605	-2.7914604750
Errors				
0.0625	AL ⁵	1.5 x 10 ⁻⁶	1.5 x 10 ⁻⁶	2.5 x 10 ⁻⁶
	AB8	-1.8 x 10 ⁻⁴	1.8 x 10 ⁻⁴	5.2 x 10 ⁻⁴
0.1	AL⁵	1.2 x 10 ⁻¹⁰	1.2 x 10 ⁻¹⁰	4.2 x 10 ⁻¹⁰
	AB8	2.2 x 10 ⁻⁸	2.2 x 10 ⁻⁹	6.3 x 10 ⁻⁹

Table 4.1 Numerical result of the non-linear stiff problem

Example 2

Second order differential equation (Okunuga[13])

The accuracy of the new method is also illustrated

$$\frac{d^2y}{dx^2} + 1001\frac{dy}{dx} + 100y = 0$$
$$y(0) = 1, y'(0) = 1$$

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The system (4.2) can be rewritten as a first – order system;

$$\frac{dy_1}{dx} = y_2 \quad y_1(0) = 1$$

$$\frac{dy_2}{dx} = -1001y_2 - 1000y_1y_2(0) = -1$$
(4.3)

Thus we obtain a 2 x 2 system of stiff IVP. The eigenvalues of the Jacobian matrix

 $\lambda_1 = -1000$

The general solution of (4.2) is $y(x) = Ae^{-x} + Be^{-1000x}$. If we impose the initial conditions in $0 \le x \le 1$ the exact solution is $y(x) = e^{-x}$.

The result of this problem using the newly derived methods are obtained at x = 1; as given in table 4.2 below.

Table 4.2: Numerical results on second order ODE at x=1

Step h	Method	y(1)	Error (y)
0.05	OK6	0.367879436	5.6 x 10 ⁻⁸
	AG6	0.36787846	1.4 x 10 ⁻⁸
	AF5	0.36787930	1.8 x 10 ⁻⁷
	AL⁵	0.36787943	5.2 x 10 ⁻⁹
0.125	AL	0.36787944	2.7 x 10 ⁻⁸
Exact So	olution	0.367879435	

It will be observed from table 4.2 above, for h=0.05 the numerical result of the problem consider reveal that the new method perform better with existing methods in the literature. The level of performing of better_____

Example 3

Jackson and Kenue[10], Cash [6], Okunuga[4]

$$y' = -y + 95z; \quad y(0) = 1$$

 $z' = -y - 97z; \quad y(0) = 1$ (4.4)

 $x \in [0, 1]$

The eigenvalues of the Jacobian matrix of the system are $\lambda_1 = -2$ and $\lambda_2 = -96$ with stiffness ratio 48.

The exact solution is given as,

$$y = (95e^{-2x} - 48e^{-96x})/47$$
$$z = (48e^{-96x} - e^{-2x})/47$$

For comparison purpose , we have the following as;

AB7, AB8 and NM9 to represent Abhulimen and Otunta "Two step third derivative methods order seven, eight and nine" respectively. F⁵ denote three-step second derivative scheme.

Method	Step size	y ₁ (/error/)	z(1) x 10 ² (/error/)
J-K	h = 0.0625	0.2725503 (3.0 x 10 ⁻⁷)	-0.2879477 (4.0 x 10 ⁻⁹)
CH4		0.2735498 (3.0 x 10 ⁻⁷)	-0.2879471 (3.0 x 10 ⁻⁹)
CH5		0.27355005 (3.0 x 10 ⁻⁸)	-0.28794742 (3.0 x 10 ⁻⁹)
AB7		0.27354004 (4.0 x 10 ⁻⁵)	-0.28796321 (6.0 x 10 ⁻⁵)
F ⁴		0.2735503 (3.0 x 10 ⁻⁷)	-0.2879477 (3.1 x10 ⁻⁷)
NM9		0.27354004 (7.9 x10 ⁻⁵)	-0.28794740 (8.3 x10 ⁻⁷)
F⁵		0.27355003 (6.4 x10 ⁻⁹)	0.28794741 (6.7 x10 ⁻⁹)

Table 4.3: Comparative analysis of result of problem 3 at x=1



AL°		0.2735501 (5.0 x 10 ⁻⁸)	-0.28794741(7.0 x 10 ⁻¹⁰)
J-K	0.03125	0.27355005 (5.0 x 10 ⁻⁷)	-0.28794742 (4.0 x 10 ⁻⁷)
CH4		0.27355003 (1.0 x 10 ⁻⁸)	-0.28794740 (1.0 x 10 ⁻¹⁰)
AL		0.2735501 (6.0 x 10 ⁻⁸)	-0.28794741(1.0 x 10 ⁻¹⁰)
AB7		0.27354004 (4.0 x 10 ⁻⁵)	-0.28796321 (6.0 x 10 ⁻⁵)
F ⁴		0.2735503 (3.0 x 10 ⁻⁷)	-0.2879477 (3.1 x10 ⁻⁷)
NM9		0.27354004 (7.9 x10 ⁻⁵)	-0.28794740 (8.3 x10 ⁻⁷)
F⁵		0.27355003 (6.4 x10 ⁻⁹)	0.28794741 (6.7 x10 ⁻⁹)
AL⁵	0.05	0.2373550 (1.1 x 10 ⁻⁷)	-0.2879947 (1.4 x 10 ⁻⁹)
AB7		0.27354004 (4.0 x 10 ⁻⁵)	-0.28796321 (6.0 x 10 ⁻⁵)
AF5		0.27354738 (2.7 x 10 ⁻⁶)	-0.28794461 (1.4 x10 ⁻⁸)
Exact so	lution	0.27355004	-0.287947411

As shown in the Table 3.1 above, the proposed method in this paper perform better than existingmethods in terms of accuracy.

5.0 CONCLUSION

The aim of this paper was to develop numerical method which provides solution to initial value problems with stiff differential equations via exponentially fitted integrators.Numerical experiments have been carried out using appropriate step size as required by each problem. Such problems which are stiff require small step size before the solution can be smooth. In general, the results from numerical experiment so presented in this paper, show that the new method perform effectively well when compared similar methods in the literature. Hence the aim and objective of this paper have been achieved.

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