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A NEW CLASS OF SECOND DERIVATIVE METHODS FOR NUMERICAL INTEGRATION OF STIFF INITIAL VALUE PROBLEMS

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ABSTRACT. A new class of four-step second derivative exponential fitting method of order six for the numerical integration of stiff initial-value problems in ordinary differential equations was constructed. The implicit method possesses free parameters which allow it to be fitted automatically to exponential functions. For the purpose of effective implementation of the newly proposed method, we adopted the mechanism which splits the method into predictor- corrector schemes. The analysis of the stability of the new method was discussed and it was found to be A-stable. Finally, some numerical experiments confirming theoretical expectations were provided. The numerical results show that the new method competes favourably with the existing methods in literature in terms of efficiency and accuracy.

Keywords and phrases: Second derivative four-step, exponentially fitted, A-stable and stiff initial value problems
2010 Mathematical Subject Classification: A80

1. INTRODUCTION

In this paper the authors focus on a class of exponentially fitted 4-step second derivative methods suitable for the approximate numerical integration of stiff systems of initial-value problem of the form

$$y' = f(x, y); y(x_0) = y_0 \tag{1}$$

on finite interval $x \in [a, b], \quad y \in R^N$
The development of numerical integrators for this class of problems has attracted considerable attention in the past decade. The reason is that most conventional numerical integration solvers cannot effectively handle stiff problems as they lack sufficient stability

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characteristics.
Implicit solvers offer stability for any time increment at the cost of a lot of computation per step. What is needed is a method that can take a long time cheaply. Exponential fitting methods offer this option. An exponential fitting method offers integration of differential equations which has large imaginary eigenvalues (Hochbruck et al. [12]). The motivating spirit behind the development of this kind of numerical integrator is that exponentially fitted formula possesses a large region of absolute stability when compared with conventional ones.
However, several authors in [1]-[20] developed A-stable numerical integrators for stiff problems whose solutions have exponential functions.
Meanwhile, the aim of this present paper is to derive a class of a four-step second derivative exponential fitting integrators of order six, which is A stable for all choices of the fitting parameters.

2. GENERAL APPROACH IN THE DERIVATION OF THE METHOD

The general multiderivative multistep method considered for the intial value problem (1) is given by;

$$\sum_{j=0}^{k} \alpha_j y_{n+j} - \Big[\sum_{i=0}^{s} h^i \sum_{j=0}^{k} \omega_{j,s} y_{n+j}^{w} \Big] = 0 \tag{2}$$

The coefficients α_j and $\omega_{j,s}$ are real constants subject to the condition $\alpha_{k=+1}$, and $\sum_{j=0}^{k} |\alpha_j| > 0$ and $\sum_{j=0}^{k} |\omega_{j,s}| > 0, \qquad s = 1, 2, \cdots$
The general approach in the derivation of the method by splitting equation (2) into predictor - corrector mode as follows;

$$\sum_{j=0}^{k} \Big[\alpha_j y_{n+j} - h\beta_j y_{n+j} + h^2 \phi_j y_{n+j} \Big] = 0 \tag{3}$$

as predictor and

$$\sum_{j=0}^{k} \alpha_j y_{n+j} - \Big[h \sum_{j=0}^{k+1} \beta_j y'_{n+j} + h^2 \sum_{j=0}^{k} \phi_j y''_{n+j} \Big] = 0 \tag{4}$$

as corrector
where the coefficients $\beta_i = \omega_{1,i}, \quad \phi_i = \omega_{2,j}$ are real constants.
It is important to remark that when deriving exponentially fitted

methods, the general approach is to allow both (3) and (4) to possess free parameters which allow them to be fitted automatically to exponential functions. **2.1 Derivation of the New Method**

To derive a four-step second derivative exponentially method of order six, we first derived the predictor, with $\alpha_k = +1$ and $\beta_k = \tau$ as free parameter, while k = 4.
Here, we generate a set of six simultaneous equations from (3) as follows;

$$\left.\begin{aligned} \alpha_0 + 1 = 0 \\ 4 - \beta_0 - \beta_2 - t = 0 \\ 8 - [(2\beta_2 + 4t) + (\phi_0 + \phi_2 + \phi_4)] = 0 \\ \tfrac{32}{3} - [(2\beta_2 + 8t) + (2\phi_2 + 4\phi_4)] = 0 \\ \tfrac{32}{3} - [(\tfrac{4}{3}\beta_2 + \tfrac{32}{3}t) + (2\phi_2 + 8\phi_4)] = 0 \\ \tfrac{128}{15} - [(\tfrac{2}{3}\beta_2 + \tfrac{32}{3}t) + (\tfrac{4}{3}\phi_2 + \tfrac{32}{3}\phi_4)] = 0 \end{aligned}\right\} \tag{5}$$

Solving for the unknown parameters, we obtain the following

$$\begin{aligned} &\alpha_0 = -1 \\ &\alpha_4 = 1 \\ &\beta_0 = (\tfrac{28}{15} - t); \quad \beta_2 = \tfrac{32}{15} \\ &\beta_4 = t \quad (free \quad parameter) \\ &\phi_0 = \tfrac{8}{9} - \tfrac{2}{3}t \\ &\phi_2 = \tfrac{112}{45}t - \tfrac{8}{3}t \\ &\phi_4 = \tfrac{16}{45} - \tfrac{2}{3}t \end{aligned}$$

Substituting the above parameters into (3), we obtain:

$$\begin{aligned} y_{n+4} = y_n + h\Big[\left(\frac{28}{15} - t\right) y_n' + \left(\frac{32}{15}\right) y_{n+2}' + t y_{n+4}'\Big] \\ + h^2\Big[\left(\frac{8}{9} - \frac{2}{3}t\right) y_n'' + \left(\frac{112}{45}t - \frac{8}{3}t\right) y_{n+2}'' + \left(\frac{16}{45} - \frac{2}{3}t\right) y_{n+4}''\Big] \end{aligned} \tag{6}$$

To obtain the exponential fitting of this method, we apply equation (6) to scalar test equation

$$y' = \lambda y', \quad y(0) = 1; \quad Re(\lambda) < 0 \tag{7}$$

We then obtain the equation

$$\frac{\overline{y}_{n+4}}{y_n} = \frac{1 + \left(\frac{28}{15} - t\right) u + \left(\frac{32}{15}u\right) \frac{y_{n+2}}{y_n} + \left(\frac{8}{9} - \frac{2}{3}t\right) u^2 + \left(\frac{112}{45} - \frac{8}{3}t\right) u^2 . \frac{y_{n+2}}{y_n}}{1 - tu - \left(\frac{16}{45} - \frac{2}{3}t\right) u^2} \tag{8}$$

This yields

$$\begin{aligned}\frac{\overline{y}_{n+4}}{y_n} &= \frac{1 + \left(\frac{28}{15} - t\right) u + \left(\frac{32}{15}u\right) e^{2u} + \left(\frac{8}{9} - \frac{2}{3}t\right) u^2 e^{2u} + \left(\frac{112}{45} - \frac{8}{3}t\right) u^2 e^{2u}}{1 - tu - \left(\frac{16}{45} - \frac{2}{3}t\right) u^2} \\ &= \overline{R}(u) say\end{aligned} \tag{9}$$

where $u = \lambda h$

Again to derive corrector of the method, we obtain the following set of 7 simultaneous equations from (4) with $\beta_{k+1} = r$ as the free parameters as follows;

$$\left.\begin{aligned} \alpha_0 + 1 &= 0 \\ 4 - \beta_0 + \beta_2 + \beta_4 + r &= 0 \\ 8 - [(2\beta_2 + 4\beta_4 + 5r) + (\phi_0 + \phi_2 + \phi_4)] &= 0 \\ \tfrac{32}{3} - \left[\left(2\beta_2 + 8\beta_4 + \tfrac{25}{2}r\right) + (2\phi_2 + 4\phi_4)\right] &= 0 \\ \tfrac{32}{3} - \left[\left(\tfrac{4}{3}\beta_2 + \tfrac{32}{3}\beta_4 + \tfrac{125}{6}r\right) + (2\phi_2 + 8\phi_4)\right] &= 0 \\ \tfrac{128}{15} - \left[\left(\tfrac{2}{3}\beta_2 + \tfrac{32}{3}\beta_4 + \tfrac{625}{24}r\right) + \left(\tfrac{2}{3}\phi_2 + \tfrac{32}{3}\phi_4\right)\right] &= 0 \\ \tfrac{256}{45} - \left[\left(\tfrac{4}{15}\beta_2 + \tfrac{128}{15}\beta_4 + \tfrac{625}{24}r\right) + \left(\tfrac{4}{3}\phi_2 + \tfrac{32}{3}\phi_4\right)\right] &= 0 \end{aligned}\right\} \tag{10}$$

Solving for the unknown parameters, we obtain the following values;

$$\alpha_0 = -1, \quad \beta_0 = \tfrac{14}{15} + \tfrac{69}{256}r, \quad \beta_2 = \tfrac{32}{15} - \tfrac{25}{16}r, \quad \beta_4 = \tfrac{14}{15} + \tfrac{75}{256}r,$$

$$\phi_0 = \tfrac{4}{15} + \tfrac{35}{128}r, \quad \phi_2 = -\tfrac{25}{32}r, \quad \phi_4 = -\tfrac{4}{15} - \tfrac{325}{128}r$$

Substituting the above values of the parameter into equation (4), we obtain the four-step corrector scheme as follows;

$$y_{n+4} = y_n + h\left[\varphi_1 y_n^{'} + \left(\frac{32}{15} - \frac{25}{16}r\right) y_{n+2}^{'} + \left(\frac{14}{15} - \frac{75}{256}r\right) y_{n+4}^{'} + r y_{n+5}^{'}\right]$$
$$+ h^2\left[\left(\frac{14}{15} + \frac{105}{384}r\right) y_n^{''} + \left(-\frac{25}{32}r\right) y_{n+2}^{''} + \left(\frac{4}{15} - \frac{975}{284}\right) y_{n+4}^{''}\right] \tag{11}$$

where,

$\varphi_1 = \left(\frac{14}{15} + \frac{69}{256}r\right)$.

As it was done in the case of the predictor, we obtain the new exponentially fitted corrector integrator of order-6 by applying equation 11 to test equation 7. So we have,

$$\frac{\overline{y}_{n+4}}{y_n} = \frac{1 + \pi_1 u + \pi_2 u.e^{2u} + ru.e^{5u} + \pi_3 u^2 + \left(-\frac{25}{32}\right) u^2 e^{5u}}{1 - \left(\frac{14}{15} + \frac{225}{768}r\right) u + \left(\frac{4}{15} - \frac{975}{384}r\right) u^2} \tag{12}$$

where,

$\pi_1 = \left(\frac{14}{15} + \frac{207}{768}r\right), \qquad \pi_2 = \left(\frac{32}{15} - \frac{25}{19}r\right), \qquad \pi_3 = \left(\frac{14}{15} + \frac{105}{384}r\right)$

3. STABILITY CONSIDERATION OF THE NEW METHOD

In this section, we shall examine the stability nature of the new method.

Remark:

It is important to know that the property of A-stability is desirable in integrators or formulas to be used in the solution of stiff problems.

Definition:

A method or an integrator is A-stable if the stability region associated with it contains the open left half of the complex plane.

Therefore, in the light of [11], [6], [5], we need to investigate the conditions which the free parameters $t(u)$ and $r(u)$ need to satisfy such that;

$$|R*(u)| < 1 \quad or \quad |\frac{y_{n+4}}{y_n}| < 1 \quad \forall \quad u; \quad Re(u) < 0 \tag{13}$$

However, necessary and sufficient condition for this inequality to hold is given by the application of the maximum modulus theorem [11] as;

(i) $|R(u)| \leq 1$ on $\quad Re(u) = 0$

(ii) $R(u)$ analytic in $Re(u) < 0$

If condition (i) holds, it follows that $R(u)$ is analytic as $u \to -\infty$ and thus, (i) and (ii) will guarantee A-stability.

Now, by analytic processes we can examine $|R*(u)| < 1$ for all $u \in (-\infty, 0]$ so that, $t(u)$ and $r(u)$ have finite limits both at $u = 0$ and $u = -\infty$ i.e., for $u \to 0$ and $u \to -\infty$.

Thus, from equation (9) and (12), we obtain the expressions for $t(u)$ and $r(u)$ respectively as follows;

$$t(u) = \frac{1 + \left(\frac{28}{15} - \frac{32}{15}e^{2u}\right)u + \frac{8}{9}u^2\left(\frac{112}{45}e^{2u} + \frac{16}{45}e^{4u}\right)u^2 - e^{4u}}{\left(1 - e^{4u}\right)u + \frac{2}{3}u^2\left(1 + e^{4u}\right) + \left(\frac{8}{3}e^{2u}\right)u^2} \tag{14}$$

and

$$r(u) = \frac{1 + \frac{32}{15}ue^{2u} + \frac{14}{15}u\left(1 + e^{4u}\right) + \left(\frac{14}{15} - \frac{4}{15}e^{4u}\right)u^2 - e^{4u}}{\left(\frac{25}{128} - e^{5u}\right)u + \left(\frac{25}{16} - \frac{225}{128}e^{4u}\right) + \left(\frac{225}{64}e^{4u} + \frac{45}{64}\right)u^2 + \frac{75}{16}u^2 - e^{2u}} \tag{15}$$

so $\lim\limits_{u \to -\infty} t(u) = \frac{4}{3}$ and $\lim\limits_{u \to 0} t(u) = -\frac{86}{115}$

Also,

$\lim\limits_{u \to -\infty} r(u) = -\frac{512}{525}$ and $\lim\limits_{u \to 0} r(u) = -\frac{1138688}{679875}$

The implication of these finite limits of t and r, is the intervals of region of stability of this method are, $t \in \left(\frac{4}{3}, \frac{86}{115}\right)$ and $r \in \left(-\frac{512}{525}, -\frac{1138688}{679875}\right) \quad \forall \quad u \in (-\infty, 0]$.

We further show that the ranges of values of t and r represent the region of absolute stability. This can be illustrated by taking a large sample N of $u \in (-\infty, 0]$ as shown in Table 1.

Table 1: Values of parameters; $t(u)$ and $r(u)$ for method of order 6

u	t	r
-10.00	1.256863	-0.743793
-20.00	1.294144	-0.855898
-30.00	1.307018	-0.894929
-50.00	1.317457	-0.926704
-100.00	1.325364	-0.950843
-200.00	1.329341	-0.963009
-1000.00	1.332534	-0.972787
-2000.00	1.332933	-0.974012
-5000.00	1.333173	-0.974748
-10000.00	1.3332553	-0.974993

From the analysis so far, as seen in Table 1, we observed that as the set of values of u in the open left half interval decreases, the corresponding values of t and r monotonically increase. We further observed that, for any value of u in the open left half plane, the values of t and r converges and bounded within the ranges $t \in \left(\dfrac{4}{3}, \dfrac{86}{115}\right)$ and $r \in \left(-\dfrac{512}{525}, -\dfrac{11387}{67988}\right)$.
Finally, it remains to investigate whether condition (ii) is $R(u) < 1$ for $Re(u) < 0$. The stability function of the predictor-corrector of the new integrator is obtained by uniting equations (9) and (12) to obtain the stability function as follows;

$$\begin{aligned}\frac{y_{n+4}}{y_n} &= \frac{1 + \pi_4 u + \pi_5 u\overline{R_1}(u) + ru\overline{R_2}(u) + \pi_6 u^2 - \frac{75}{16} r u^2 \overline{R_1}(u)}{1 - \left(\frac{14}{15} + \frac{225}{128} r\right) u + \left(\frac{4}{15} + \frac{225}{64} r\right) u^2} \\ &= R*(u)\end{aligned} \tag{16}$$

where,
$\pi_4 = \left(\frac{14}{15} - \frac{25}{128} r\right)$, $\qquad \pi_5 = \left(\frac{32}{15} - \frac{25}{16} r\right)$, $\qquad \pi_6 = \left(\frac{14}{15} - \frac{45}{64} r\right)$,

$$\frac{y_{n+2}}{y_n} = \overline{R_1}(u) = \left[\frac{\overline{y}_{n+4}}{y_n}\right]^{\frac{1}{2}} \quad \text{and} \quad \frac{y_{n+5}}{y_n} = \overline{R_2}(u) = \left[\frac{\overline{y}_{n+4}}{y_n}\right]^{\frac{5}{4}}$$

When we test for values of $u \in (-\infty, 0]$ within the range of parameters a and r above, we established that $|R*(u)| < 1$ for all $u \in (-\infty, 0]$. The region of stability function of the new method is shown in Figure 1, confirming that our method is A-stable.
However, we remark that all class of second derivative methods of at least order four, five and six are consistent and A-stable. They are applicable to both non-linear and linear stiff initial value problems.

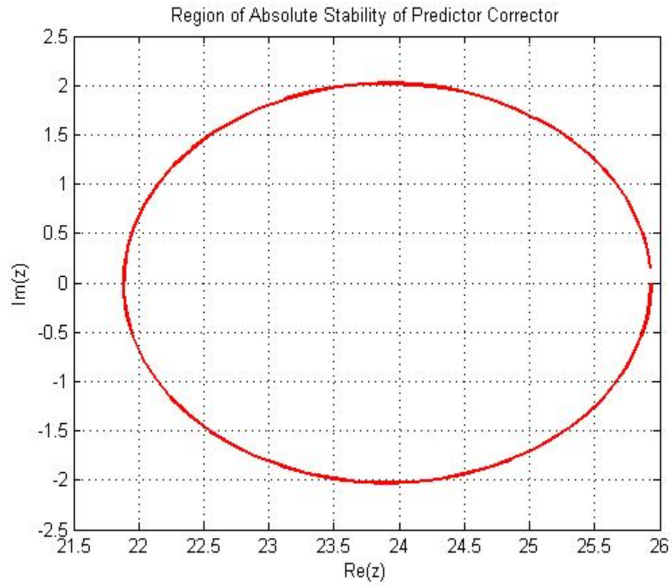

Fig. 1. Region of Absolute Stability of Predictor Corrector

4. NUMERICAL EXAMPLES

In this section, we shall apply the new method to solve some standard stiff problems. We shall compare the numerical results obtained by the new method with other existing methods which have been used in solving the same set of problems. All computations were carried out by digital computer using FORTRAN 77 package on double precision.
Now, for the purpose of comparative analysis of performance of the new integrator on the various numerical examples, we denote F6 as the new method, CH4 and CH5 - [3] methods of order 4 and 5 respectively, J-K - [14] method, F^4 - [20] method of Order 4, F^5 - [2] method of Order 5, AB8-[1], NM9- [8], AF5- [5], AG6 - [6], A6 - [3], BDF1, BDF2 - [19], AB6- [4].

Example 1

Consider the non-linear stiff problem [19]

$$y_1^{'} = -0.013y_1 + 1002y_1y_3, \qquad y_1(0) = 1$$
$$y_2^{'} = 2500y_2y_3, \qquad y_2(0) = 1$$
$$y_3^{'} = 0.013y_1 - 1020y_1y_3 - 2500y_2y_3, \qquad y_3(0) = 0$$

The eigenvalues of the system are given by $\lambda_1 = 0, \quad \lambda_2 = -0.00928572$ and $\lambda_3 = -3500.003714$. The stiffness ratio is 376923.14. The exact solution is given by $y_j^{'} = C_j + D_je^{\lambda 2x}, \quad j = 1, 2, 3$, where C_j and D_j

are determined using the initial value conditions. The numerical results of problem 1 are displayed in Table 2.

Table 2: Maximum absolute error in problem 1 at $x = 1$.

Step length h	Methods	$y_1(1)$	$y_2(1)$	$y_3(1)$
	Errors	**Errors**	**Errors**	**Errors**
0.0625	AB8	-1.8×10^{-4}	1.8×10^{-4}	5.2×10^{-4}
	F6	$\mathbf{1.7 \times 10^{-14}}$	$\mathbf{5.7 \times 10^{-13}}$	$\mathbf{4.0 \times 10^{-13}}$
	F5	1.6×10^{-10}	1.6×10^{-10}	1.6×10^{-10}
	AB6	2.5×10^{-10}	2.0×10^{-10}	4.3×10^{-10}
0.1	AB8	-2.2×10^{-8}	2.2×10^{-9}	6.3×10^{-9}
	F6	$\mathbf{1.7 \times 10^{-14}}$	$\mathbf{5.7 \times 10^{-13}}$	$\mathbf{4.0 \times 10^{-13}}$
	F5	2.4×10^{-10}	2.4×10^{-10}	2.2×10^{-10}
	AB6	1.8×10^{-10}	1.5×10^{-10}	4.5×10^{-10}
Exact solution			1.0092403605	2.7914604750

Remark: The new second derivative exponentially fitted method of order 6 (F6) competes favourably in terms of accuracy of [19] and [17] method of order 4 as seen in Table 2.

Example 2

We consider the linear stiff problem from [11] and [12].

$$y' = -y + 95z, \qquad y(0) = 1$$
$$y' = -y - 97z, \qquad y(0) = 1 \qquad x \in [0, 1]$$

The eigenvalues of the Jacobian matrix of the system are $\lambda_1 = -2$ and $\lambda_2 = -96$. The exact solution is given as

$$y = \frac{\left(95e^{-2x} - 48e^{-95x}\right)}{47}$$
$$y = \frac{\left(48e^{-96x} - e^{-2x}\right)}{47}$$

The numerical results are displayed on Table 3.

Table 3: Comparative analysis of result of Example 2 at $x = 1$.

Step length h	Methods	$y(1)(\|error\|)$	$Z(1) \times 10^2(\|error\|)$
0.0625	CH4	$0.2735498(3.0 \times 10^{-7})$	$-0.2879471(4.0 \times 10^{-9})$
	CH5	$0.27554005(3.0 \times 10^{-8})$	$-0.2879274(3.0 \times 10^{-9})$
	J-K	$0.2735523(1.0 \times 10^{-8})$	$-0.2879477(4.0 \times 10^{-9})$
	F^4	$0.2735503(3.0 \times 10^{-7})$	$-0.2879477(3.1 \times 10^{-7})$
	F^5	$0.2735523(6.4 \times 10^{-9})$	$-0.2879441(6.7 \times 10^{-9})$
	AF^5	$0.27354958(4.5 \times 10^{-7})$	$-0.28794694(4.7 \times 10^{-9})$
	F6	$\mathbf{0.27354997(3.0 \times 10^{-8})}$	$\mathbf{-0.2879471(1.4 \times 10^{-9})}$
	NM9	$0.27354656(7.8 \times 10^{-5})$	$-0.29794811(3.7 \times 10^{-5})$
	BDF1	$0.27355004(1.91 \times 10^{-9})$	$-0.2879474(2.01 \times 10^{-9})$
	BDF2	$0.036994834(2.73 \times 10^{-1})$	$-0.00038942(2.49 \times 10^{-9})$
0.03125	CH4	$0.2735498(3.0 \times 10^{-7})$	$-0.2879471(4.0 \times 10^{-9})$
	J-K	$0.2735523(1.0 \times 10^{-8})$	$-0.2879477(4.0 \times 10^{-9})$
	AB8	$0.2735523(1.0 \times 10^{-8})$	$-0.2879477(4.0 \times 10^{-9})$
	F^4	$0.2735503(3.0 \times 10^{-7})$	$-0.2879477(3.1 \times 10^{-7})$
	NM9	$0.27354656(7.8 \times 10^{-5})$	$-0.29794811(3.7 \times 10^{-5})$
	F6	$\mathbf{0.27354997(3.0 \times 10^{-8})}$	$\mathbf{-0.2879471(1.4 \times 10^{-9})}$
	BDF1	$0.27355004(1.91 \times 10^{-9})$	$-0.2879474(2.01 \times 10^{-9})$
	BDF2	$0.036994834(2.73 \times 10^{-1})$	$-0.00038942(2.49 \times 10^{-9})$
Exact solution		0.2735004	-0.287947411

Remark: From Table 3, the numerical results revealed that our method of order 6, competes favourably in terms of accuracy when compared with other existing methods.

Example 3

Consider a linear stiff problem [5]

$$y^{''} + 1001y^{'} + 1000y = 0$$

$$y(1) = 1 \qquad y^{'}(0) = 1,$$

The eigenvalues of the Jacobian matrix of the system are $\lambda_1 = -1$ and $\lambda_2 = -1000$. The general solution is $y(x) = Ae^{-x} + Be^{-1000x}$. If when we invoke the initial conditions in $x \in [0, 1]$ the exact solution becomes $y(x) = e^{-x}$.
Numerical results obtained at $x = 1$ using the newly derived method are shown on Table 4.

Table 4: Numerical results on second order (ODE) at $x = 1$.

Step length h	Methods	$y(1)$	Absolute Error (y)
0.05	F5	0.36787944	5.2×10^{9}
	AG6	0.36787846	1.4×10^{-8}
	AF5	0.36787930	1.8×10^{-7}
	F6	**0.36787930**	$\mathbf{8.9 \times 10^{-8}}$
0.125	F5	0.367879442	2.7×10^{-8}
	F6	**0.367879450**	$\mathbf{6.0 \times 10^{-8}}$
Exact solution		0.36789435	

Remark: From the above results, our scheme competes favourably when compared with other existing schemes.

5. CONCLUDING REMARK

From the results presented so far in this paper we conclude and affirm that the new method is A-stable and capable of solving systems of stiff problems for which exponential fitting are applicable. We also observed that the method possesses high accuracy and stability properties when compared with existing methods in the literature that were used to solve the same set of problems.

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