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MAXIMUM ORDER SECOND DERIVATIVE HYBRID MULTI-STEP METHODS FOR INTEGRATION OF INITIAL VALUE PROBLEMS IN ORDINARY DIFFERENTIAL EQUATIONS

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ABSTRACT
In this paper, we propose a k-step second derivative hybrid linear multistep formula of maxima order for solution of stiff and non-stiff initial value problems in ordinary differential equations. The method is motivated by second derivative formulas:

$$y_{n+k} = y_{n+k-1} + h\sum_{j=0}^{k}\beta_j y'_{n+j} + h\beta_r y'_{n+k-r} + h^2\rho y''_{n+k}\text{ , } 0<r<1\text{ , step size h}$$

in which the control parameter r is specified in advance.and the step size is h.
We, in our attempt, allowed this parameter r to assume its exact value by solving the resulting non-linear equations of the co-efficients. The resultant formulas are A-stable and of maxima order 2k+1 when k is even and 2k+2 when k is odd. The formulas are derived, analyzed and implemented for k=1 and k=2. The experimental results show a high degree of accuracy.

1. INTRODUCTION

The solution of initial value problems of ordinary differential equations of the form :

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

where y, f ∈ R^n, x ∈ [a,b], has been discussed by various authors (Lambert (1973), Gear (1971)). Enright (1974(a)) developed the second derivative multi-step formulas:

$$y_{n+k} = y_{n+k-1} + h\sum_{j=0}^{k}\beta_j y'_{n+j} + h^2\rho y''_{n+k} \tag{1.2}$$

to solve problems of the form (1.1), in which the parameters β's and ρ_0 determine the order of accuracy of the method. But Enright and Hull (1975) indicated that the second derivative code was relatively inefficient.
Ademiluyi (1987) considered how this inefficiency might be improved and came up with the second derivative hybrid formulas:

$$y_{n+k} = y_{n+k-1} + h\sum_{j=0}^{k}\beta_j y'_{n+j} + h\beta_r y'_{n+k-r} + h^2\rho y''_{n+k} \quad 0<r<1, \text{ step size h} \qquad (1.3)$$

The idea is to include more analytic properties of y and f at some on-step and off-step points.

In his approach, the value of the controlling parameters r is specified in advance in order to reduce the complexity of the resulting non-linear equations to be solved at the expense of the order of accuracy. However in this paper, we optimized the order of the accuracy of the scheme by allowing the parameters to take their exact values which will guarantee adequate stability and convergence properties and also ensure acceptable results. The computation of these parameters is discussed in the next section.

2. DETERMINATION OF PARAMETERS

In this section we give an outline of the calculation of the parameters β_j's, β_r, ρ and r for cases k=1 and k=2. The same procedure can be used for k>2.

Now, define an operator Ł associated with the scheme (1.3) as:

$$L[y(x),h] = y(x_{n+k}) - y(x_{n+k-1}) - h\sum_{j=0}^{k}\beta_j y'(x_{n+j}) - h\beta_r y'(x_{n+k-r}) - h^2\rho y''(x_{n+k}) \qquad (2.1)$$

for $y(x)\in C^{q+1}[a,b]$, $y(x_{n+p}) = y(x_n + hp) \quad a,b,p\in R$

If y(x) represents the true solution of (1.1) and we adopt Taylor series expansion of functions $y(x_{n+k})$, $y(x_{n+k-1})$ and the derivatives $y'(x_{n+j})$, $j=0(1)k$, $y'(x_{n+k-r})$ and $y''(x_{n+k})$ about $x=x_n$ we get ; for k ≥ 1

$$y(x_{n+k}) = \sum_{s=0}^{k}\frac{\{h^s y^{(s)}(x_n)\}k^s}{s!} \; ; \quad y^{(0)} = y \qquad (2.2)$$

$$y(x_{n+k-1}) = \sum_{s=0}^{k}\frac{\{h^s y^{(s)}(x_n)\}(k-1)^s}{s!} \qquad (2.3)$$

$$y'(x_{n+j}) = \sum_{s=1}^{k}\frac{\{h^{s-1} y^{(s)}(x_n)\}j^{s-1}}{(s-1)!} \; ; \quad j = 0,1,\ldots k \qquad (2.4)$$

$$y'(x_{n+k-r}) = \sum_{s=1}^{k} \frac{\{h^{s-1} y^{(s)}(x_n)\}(k-r)^{s-1}}{(s-1)!} \; ; \qquad (2.5)$$

$$y''(x_{n+k}) = \sum_{s=2}^{k} \frac{\{h^{(s-2)} y^{(s)}(x_n)\} k^{s-2}}{(s-2)!} \; ; \qquad (2.6)$$

Substituting (2.2) - (2.6) into (2.1) and combining terms of equal powers of h, we get:

$$L[y(x),h] = C_0 y(x_n) + C_1 h y^{(1)}(x_n) + C_2 h^2 y^{(2)}(x_n) + \ldots + C_q h^q y^{(q)}(x_n) + C_{q+1} h^{q+1} y^{(q+1)}(x_n) + 0(h^{q+2}) \qquad (2.7)$$

where

$$\begin{aligned}
C_0 &= 0 \\
C_1 &= 1 - \sum_{j=0}^{k} \beta_j - \beta_r \; ; \\
C_2 &= \frac{1}{2!}\left[k^2 - (k-1)^2\right] - \sum_{j=0}^{k} j\beta_j - (k-r)\beta_r - \rho \; ; \\
C_q &= \frac{1}{q!}\left[k^q - (k-1)^q\right] - \frac{1}{(q-1)!}\left[\sum_{j=0}^{k} j^{q-1}\beta_j + (k-r)^{q-1}\beta_r\right] - \rho\frac{k^{q-2}}{(q-2)!}
\end{aligned} \qquad (2.8)$$

$$q \geq 2$$

The values of the unknown parameters β_j's, β_r, ρ and r are obtained by setting:

$$c_q = 0, \; q = 1(1)k+3 \qquad (2.9)$$

with the principal truncation error

$$\frac{1}{(q-1)!} C_{q+1} h^{q+1} y^{(q+1)}(x_n) + 0(h^{q+2}) \qquad (2.10)$$

(a) <u>First Step Method</u>

For case k=1, (2.8) - (2.10) yield the following system of non-linear equations

$$\beta_r + \beta_1 + \beta_0 = 1$$

$$(1-r)\beta_r+\beta_1+\rho = 1/2$$
$$(1-r)^2\beta_r+\beta_1+2\rho = 1/3 \qquad (2.11)$$
$$(1-r)^3\beta_r+\beta_1+3\rho = 1/4$$

A cursory look at (2.11) reveals that the parameters exceed the number of equations, therefore solving (2.11) in terms of a free parameter β_0 gives

$$r = \frac{3}{4}\frac{(1-4\beta_0)}{(1-3\beta_0)}$$
$$\beta_r = \frac{16}{27}\frac{(1-3\beta_0)^3}{(1-4\beta_0)^2} \qquad (2.12)$$
$$\beta_1 = \frac{1}{27}\frac{(11-99\beta_0+216\beta^2)}{(1-8\beta_0+16\beta_0^2)}$$
$$\rho = -\frac{1}{18}\frac{(1-6\beta_0)}{(1-4\beta_0)}$$

The scheme is optima when the free parameter β_0 is set at zero. Using this value of β_0 in (2.12) we have

$$R = 3/4$$
$$\beta_r = 16/27 \qquad (2.13)$$
$$\beta_1 = 11/27$$
$$\rho = -1/18$$

These values satisfy (2.7) with

$$C_0=C_1=C_2=C_3=C_4=0 \text{ and } C_5 = -1/1920 \qquad (2.14)$$

Hence we obtained a fourth order optima second derivative method of the form:

$$y_{n+1} = y_n + \frac{h}{27}\left(11y'_{n+1}+16y'_{n+r}\right) - \frac{h^2}{18}y''_{n+1} \qquad (2.15)$$

with the principal error term $T_5 = -1/1920\, h^5$

b) Two-Stage Method

Case k=2

for k=2, equations (2.8)-(2.10) now yield

$$\begin{aligned}
&\beta_r + \beta_2 + \beta_1 + \beta_0 = 1\\
&(2\text{-}r)\ \beta_r + 2\beta_2 + \beta_1 + \rho = 3/2\\
&(2\text{-}r)^2\ \beta_r + 4\beta_2 + \beta_1 + 4\rho = 7/3\\
&(2\text{-}r)^3\ \beta_r + 8\beta_2 + \beta_1 + 12\rho = 15/4\\
&(2\text{-}r)^4\ \beta_r + 16\beta_2 + \beta_1 + 32\rho = 31/5
\end{aligned} \qquad (2.16)$$

Just as the case k=1 leads to a system of non-linear equations with more parameters than the number of equations. We also have the system of non – linear equations with more parameters than the number of equations. So, we also express other parameters in terms of a free parameter β_0 to get

$$\begin{aligned}
r &= \frac{3}{5}\frac{(1+160\beta_0)}{(1+48\beta_0)}\\
\beta_r &= \frac{125}{216}\frac{(1+48\beta_0)^4}{(1-120\beta_0)(1+160\beta_0)^2}\\
\beta_2 &= \frac{8+3981\beta_0+377280\beta_0^2}{27(1+160\beta_0)^2}\\
\beta_1 &= (1-\beta_0)-\left\{\frac{125(1+48\beta_0)^4}{216(1-120\beta_0)(1+160\beta_0)^2}+\frac{8+3981\beta_0+377280\beta_0^2}{27(1+160\beta_0)^2}\right\}\\
\rho &= -\frac{1}{36}\frac{(1+552\beta_0)}{(1+160\beta_0)}
\end{aligned} \qquad (2.17)$$

To obtain the method of maxima order, we set $\beta_0 = 0$, thus we have

$$\begin{aligned}
&R = 3/5\\
&\beta_r = 125/216\\
&\beta_2 = 8/27\\
&\beta_1 = 1/8\\
&\rho = -1/36
\end{aligned} \qquad (2.18)$$

Substituting (2.18) into (2.7) yields

$C_0=C_1=C_2=C_3=C_4=C_5=0$ and $C_6= -1/36000$ (2.19)

Thus, the resultant fifth order maxima method is of the form:

$$y_{n+2} = y_{n+1} + \frac{h}{216}\left(64y'_{n+2} + 27y'_{n+1} + 125y'_{n+\frac{7}{5}}\right) - \frac{h^2}{36}y''_{n+2} \quad (2.20)$$

with the principal error term $T_6 = -1/3600\, h^6$

3. CONVERGENCE AND STABILITY ANALYSIS

We, in this section, discuss the stability and convergence properties of the integration scheme (1.3). We limit the discussion to the case k=1 since the procedure is the same for cases k>1.

By applying the integration formula (2.15) to the standard stability test initial value problem:

$$y^1 = \lambda y, \quad y(x_0) = y_0 \quad (3.1)$$

where λ is a complex constant satisfying $Re(\lambda)<0$, we have

$$y_{n+1} = y_n + \frac{11}{27}\bar{h}y_{n+1} + \frac{16}{27}\bar{h}y_{n+\frac{1}{4}} - \frac{h^2}{18}y''_{n+1} \quad (3.2)$$

where

$\bar{h} = \lambda h$

Approximating $y_{n+\frac{1}{4}}$ by

$$y_{n+\frac{1}{4}} = \left(1 + \frac{\bar{h}}{4} + \frac{\bar{h}^2}{2!4^2} + \frac{\bar{h}^3}{3!4^3} + 0(\bar{h})^4\right)y_n \quad (3.3)$$

and substituting it into (3.2) yields, after simplification

$$y_{n+1} = \phi(\bar{h})y_n \quad (3.4)$$

where

Here the exact solutions are:

$$ {}^{1}y = -1.499875 \exp(-0.5x) + 0.499875 \exp(-2000.5x) + 1 $$
$$ {}^{2}y = -2.99975 \exp(-0.5x) - 0.00025 \exp(-2000.5x) + 1 $$

The numerical results of examples 1 and 2 are as shown in tables 1 and 2 respectively. Figures 1 and 2 also show the plot of exact solution $y(x_n)$ and the numerical approximation y_n against x_n. The closeness of the exact solution and the numerical solution as the integration process continues is a proof of high accuracy of the method.

5. CONCLUSION.

An accurate k – step hybrid second derivative linear multi step formula of maxima order for solution of stiff and non – stiff ordinary differential equations is developed, analysed and implemented. Two test examples have been solved to demonstrate the accuracy of the method for k = 1 and the results as shown in tables I and II are plotted.

Algorithms of maximum order 2k + 1 when k is even, and 2k + 2 when k is odd are achieved. This is as against order 2k when k is even and 2k + 1 when k is odd for the parent formula. Fig I in particular confirms the high order of accuracy of the method.

TABLE 1

NUMERICAL SOLUTION OF PROBLEM (4.1) OVER THE INTERVAL [0,1] WITH THE BASIC STEP SIZE h = 0.1.

h	y_E	y_n	E_n	NOFHS
0.100000D00	0.453999D-4	-0.188083D1	0.214454D-1	3
0.500000D-1	0.673795D-2	-0.657766D0	0.200536D-1	3
0.250000D-1	0.820850D-1	-0.122095D0	0.197436D-1	3
0.125000D-1	0.286505D-00	0.261286D00	0.168208D-1	3
0.625000D-2	0.535261D-00	0.535235D00	0.124074D-1	3
0.3125000D-2	0.731616D00	0.731615D00	0.784083D-2	3
0.156250D-2	0.855345D00	0.855345D00	0.443528D-2	3
0.781250D-3	0.924849D00	0.92449D00	0.236270D-2	3
0.390625D-3	0.961691D00	0.961691D00	0.121590D-3	3
0.19531D-3	0.980658D00	0.980658D00	0.619892D-3	3
0.38833D-4	0.993138D00	0.993138D00	0.156871D-3	3

$$\phi(\bar{h}) = \frac{1 + \frac{16\bar{h}}{27} + \frac{4\bar{h}^2}{27} + \frac{\bar{h}^3}{27X2!}}{1 - \frac{11\bar{h}}{27} + \frac{4\bar{h}^2}{18}} \quad (3.5)$$

Now, imposing the condition

$$\left|\phi(\bar{h})\right| < 1, \text{ on } (3.5) \quad (3.6)$$

we obtain

$$\mathrm{Re}(\bar{h}) < 0 \quad (3.7)$$

Showing that the scheme is A-stable. But A-stable methods are necessarily convergent (Lambert (1973)), hence the scheme is convergent.

4. NUMERICAL EXPERIMENT

The scheme (2.15) is used to solve two sample problems. In sample problem 1, we used a variable step size h starting with h=0.10 while in example 2, we used a constant step size with h=0.50.

Example 1.

$$y^{I} = -100y, \quad y(x_0) = 1, \quad x \in [0,1] \quad (4.1)$$

The exact solution to problem (4.1) is

$y(x) = e^{-100x}$ and the time constant is 0.01.

Example 2.

$$^{1}y^{1} = -2000\,^{1}y + 999.75\,^{2}y + 1000.25$$
$$^{2}y^{1} = {}^{1}y - {}^{2}y$$

with initial conditions.

$$^{1}y(0) = 0 \qquad (4.2)$$
$$^{2}y(0) = -2$$

$$x \in [0,10]\,;\; y' = \left[{}^{1}y',\, {}^{2}y'\right]^{T}, \quad y = \left[{}^{1}y,\, {}^{2}y\right]^{T}$$

TABLE 2
NUMERICAL SOLUTION OF PROBLEM (4.2) WITH STEPSIZE h = 0.5 AND TOLERANCE 10^{-3} USING HYBRID FORMULA.

x	$1y_E$	$2y_E$	$1y_n$	$2y_n$	e_1	e_2
0.00	0.1681038245	-1.336207649	-0.638918D-7	-0.20096D1	0.62546D-10	-0.195980D-3
0.50	0.09027982676	-0.8194403465	-0.168268D00	-0.133752D1	-0.164725D-4	-0.130935D-3
1.00	0.2915092167	-0.4169815666	0.903685D-1	-0.320243D0	0.884654D-5	-0.802970D-4
1.50	0.4482268232	-0.1035463537	0.291795D0	-0.417390D0	0.285650D-4	-0.406600D-4
2.00	0.5702786178	-0.1405572356	0.44856D0	-0.103645D0	0.439218D-4	-0.101465D-4
2.50	0.665332651	0.3306653021	0.570838D0	0.140695D0	0.558816D-4	0.137732D-4
3.00	0.7393608066	0.4787216131	0.665985D0	0.330990D0	0.651960D-4	0.32401D-4
3.50	0.7970139921	0.5940279841	0.640085D0	0.479191D0	0.724500D-4	0.46910D-4
4.00	0.8419143381	0.6838286761	0.797795D0	0.594610D0	0.780994D-4	0.58208D-4
4.50	0.8768827627	0.7537655254	0.847739D0	0.684499D0	0.824992D-4	0.670084D-4
5.00	0.9041161992	0.8082323983	0.677742D0	0.684499D0	0.859258D-4	0.738615D-4
5.50	0.9253256208	0.8506512417	0.905002D0	0.754504D0	0.885944D-4	0.791987D-4

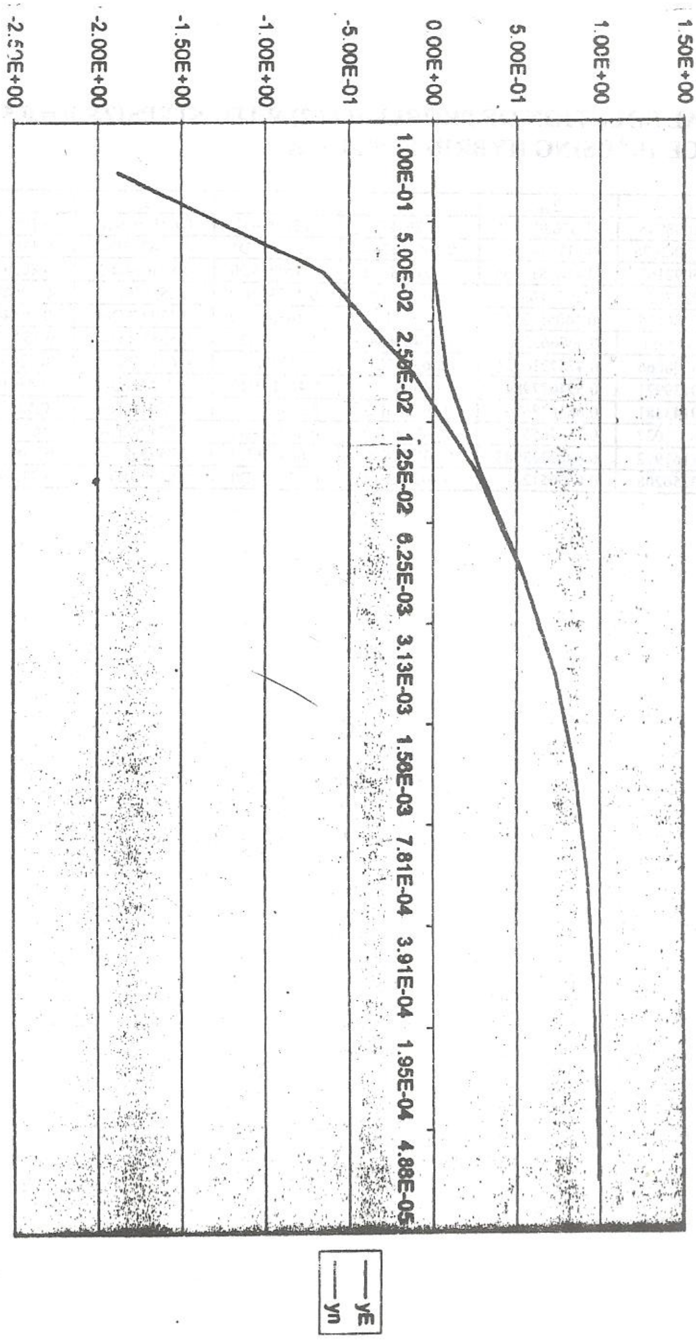
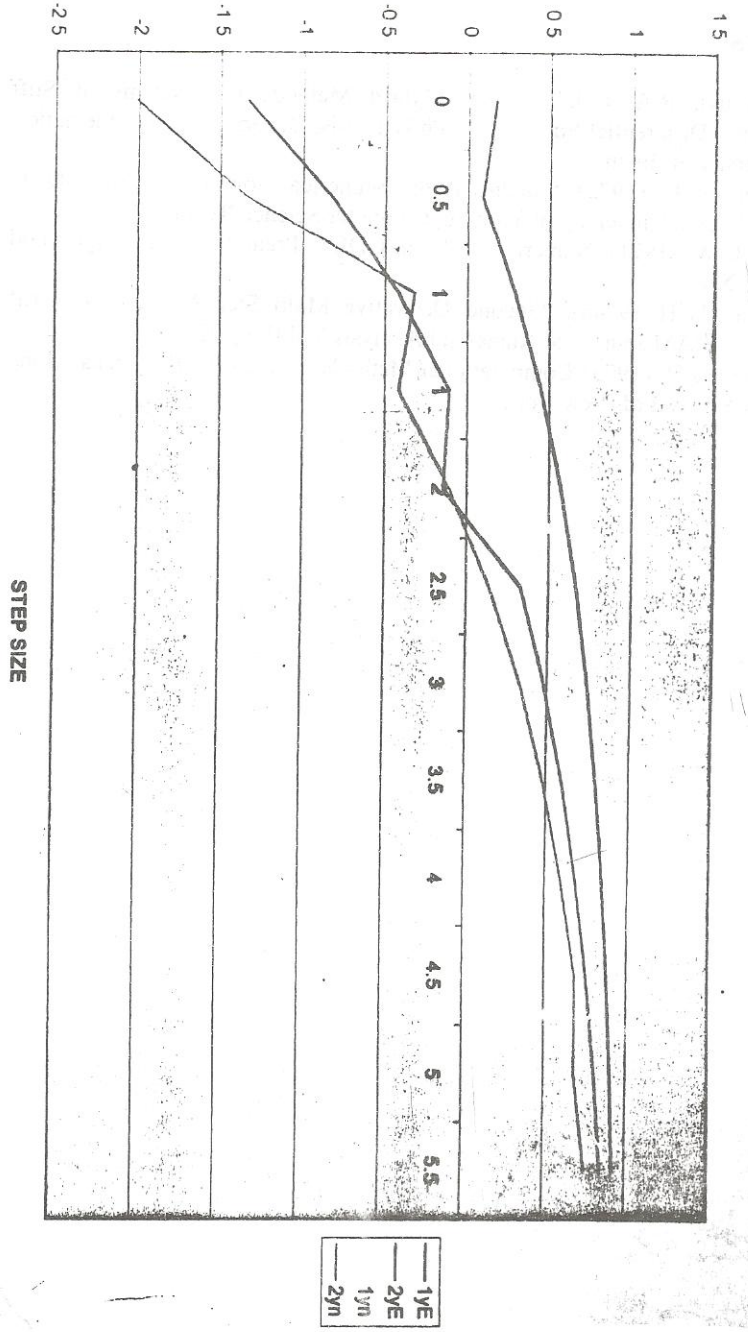


FIG 1

NUMERICAL SOLUTION OF PROBLEM (4.1) OVER THE INTERVAL (0,1) WITH THE BASIC STEP SIZE H = 0.1 USING HYBRID FORMULA (2.15)

FIG 2

NUMERICAL SOLUTION OF PROBLEM (4.2) WITH STEP SIZE H = 0.5 AND TOLERANCE 10^{-3} USING HYBRID FORMULA (2.15)



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