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A COMPARATIVE STUDY OF THE SPECIAL MULTISTEP METHODS FOR THE NUMERICAL INTEGRATION OF $Y''=f(x,y)$

By

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ABSTRACT

Special multistep methods based on numerical integration have been derived in Henrici [6] for the numerical solution of the differential equation $Y''=f(x,y)$. In this paper, methods based on Numerical Differentiation are derived and their regions of absolute stability of some classes of special multistep methods is presented.

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Keywords : Multi-step methods, Special Multi step methods, Numerical Differentiation, Initial Value Problem, Absolute stability.

1. Introduction. An extensive study of the single step and multistep methods for the first order initial value problem of ordinary differential equations has been made by several researchers and a detailed treatment of the subject has been provided by many authors ([1], [4],[6],[7],[10],[11]). An introductory treatment of various topics of Numerical Analysis can be found in [3]. Dahlquist ([1],[2]) has established the criteria for the stability and convergence of multistep methods for the solution of first order initial value problems. Special multistep methods based on numerical integration such as Adams-Bash forth methods, Adoms-Moulton methods and methods based on numerical differentiation for solving first order differential equations have been derived in Henrici [6] and Gear [4]. The methods based on numerical differentiation for first order differential equations have been shown to be stiffly stable by Gear [4], High order stiffly stable methods were considered by Jain [7]. The methods based on numerical differentiation for the first order equations are termed as Numerical Differentiation Methods by Klopfenstein [9]. Numerical differentiation methods with an off-step point were considered by Gragg and Statter [5]. High order numerical differentiation type formulas with one or more off-step points were derived in [12] and [13]. The objective of introducing an off-step point was to increase the order of the method for a given step number. The motivation for the work carried out in this paper arises from the methods based on numerical differentiation for the first order differential equations, Special multistep methods based on numerical integration for the solution of the special second order differential equations have been derived in Henrici [6]. Intial value technique for a class of non-linear singular perturbation problems were considered in [8]. Generalized multistep methods for special second order differential equations were considered in [14].

Analogous to the methods based on numerical differentiation for first order diffrential equation discussed in Henrici [6], we have derived the methods based on numerical differentiation for the special second order differential equation. In Henrici [6] methods based on numerical integration have been derived by integrating $Y''=f(x,y)$ twice and replacing the function $f(x,y)$ by an interpolating polynomial. Some of the special methods that arise are Stomer's methods, Cowell's methods etc. We have derived Special Multistep methods by replacing $Y(x)$ on the left hand side of $Y''(x)=f(x,y)$ by an interpolating polynomial and differentiating twice. We have studied the resulting implicit methods and a class of explicit methods. The interesting feature of the implicit methods and explicit methods is that they contain only one derivative term, where as the Stomer's methods and Cowell's methods based on numerical integration contain more derivative terms. Obviously, application of the implicit and explicit methods is comparatively economical as there is only one function evaluation in each of them and more function evaluation in Stormer's and Cowell's methods. It is found that the implicit and explicit methods have order $(k-1)$. The region of absolute stability of the methods were derived are exhibited in figures 1 to 10.

2. General Linear Multistep Methods for Special Second Order Differential Equations. The special second order differential Equation

$$Y''=f(x,y),\ Y(0)=Y_0,\ Y'(0)=Y'_0 \tag{1}$$

often arises in a number of applications such as mechanical problems without dissipation. A general linear multistep method of step number k for the numerical solution of (1) is give by

$$Y_{n+1}=\sum_{j=1}^{k}a_j y_{n+1-j}+h^2\sum_{j=0}^{k}b_j y_{n+1-j} \tag{2}$$

where a_j, b_j are constants and h is the step size.

Introducing the polynomials

$$\rho(\xi)=\xi^k-\sum_{j=1}^{k}a_j\xi^{k-1} \text{ and } \sigma(\xi)=\sum_{j=1}^{k}b_j\xi^{k-j} \tag{3}$$

(2) can be written as $\rho(E)Y_{n-k+1}-h^2\sigma(E)y''_{n-k+1}=0$, (4)

where E is the shift operator defined by $E(y_n)=y_{n+1}$.

Applying (4) to $y''=\lambda y$, we get the characteristic equation

$$\rho(\xi)-\bar{h}\sigma(\xi)=0,\ \text{where } \bar{h}=\lambda h^2 \tag{5}$$

The roots ξ_i of the characteristic equation (5) and $\bar{h}$ are in general, complex and the region of absolute stability is defined to be the region of the complex $\bar{h}$ -plane such that the roots of the characteristic equation (5) lie within the unit circle whenever $\bar{h}$ lies in the interior of the region. If we denote the region of absolute stability of R and its boundary by ∂R, then the locus of ∂R is given by

$$\bar{h}(\theta) = \rho(e^{i\theta})/\sigma(e^{i\theta}), 0 \le \theta \le 2\pi . \qquad (6)$$

3. Derivation of the Methods. Let $p(x)$ be the backward difference interpolating polynomial of $Y(x)$ at the $(k+1)$ abscissas $x_{n+1}, x_n, \ldots, x_{n-k+1}$. Then $p(x)$ is given by

$$p(x) = \sum_{m=0}^{k} (-1)^m \binom{-s}{m} \nabla^m y_{n+1}, \; s = (x - x_{n+1})/h . \qquad (7)$$

Differentiating (7) twice with respect to x, we get

$$p''(x) = \left(\frac{1}{h^2}\right) \sum_{m=0}^{k} \frac{d^2}{ds^2}\left[(-1)^m \binom{-s}{m}\right] \nabla^m y_{n+1} .$$

Replacing $y''(x)$ by $p''(x)$ in the equation (1) and putting $x = x_{n+1-r}$, i.e. $s = -r$, we get

$$\left(\frac{1}{h^2}\right) \sum_{m=0}^{k} \frac{d^2}{ds^2}\left[(-1)^m \binom{-s}{m}\right]\Big|_{s=-r} \nabla^m y_{n+1} = f_{n+1-r} .$$ This takes the form

$$\sum_{m=0}^{k} \delta_{r,m} \nabla^m y_{n+1} = h^2 f_{n+1-r} , \qquad (8)$$

where $$\delta_{r,m} = \frac{d^2}{ds^2}\left[(-1)^m \binom{-s}{m}\right]. \qquad (9)$$

4. Generating Function for the Coefficients $\delta_{r,m}$.

Let $$D_{r,t} = \sum_{m=0}^{\infty} \delta_{r,m} t^m . \qquad (10)$$

Substituting (9) in (10), we get

$$D_{r,t} = \sum_{m=0}^{\infty} (-t)^m \frac{d^2}{ds^2}\left({}^{-s}c_m\right) \text{ at } s=-r$$

$$= \frac{d^2}{ds^2} \sum_{m=0}^{\infty} (-t)^m \left({}^{-s}c_m\right) \text{ at } s=-r$$

$$= \frac{d^2}{ds^2} (1-t)^{-s} \text{ at } s=-r$$

$$= \frac{d^2}{ds^2} e^{-s\log(1-t)} \text{ at } s=-r$$

$$= (1-t)^{-s}[\log(1-t)]^2 \; s=-r.$$

Therefore

$$\sum_{m=0}^{\infty} \delta_{r,m} t^m = (1-t)^{-s}[log(1-t)]^2 \text{ at } s=-r. \quad (11)$$

5. Implicit Methods. Putting $r=0$ in (8), we get the implicit method.

$$\sum_{m=0}^{k} \delta_{0,m} \nabla^m y_{n+1} = h^2 f_{n+1}, \quad (12)$$

where from (12), $\delta_{0,m}$ is the coefficient of t^m in the expansion of $[\log(1\text{-}t)]^2$ in powers of t. The coefficient $\delta_{0,m}$ are tabulated below:

Table 1. Coefficients $\delta_{0,m}$: $m=0(1)8$

m	0	1	2	3	4	5	6	7	8
$\delta_{0,m}$	0	0	1	1	11/12	5/6	137/180	7/10	1089/1680

Difference in (12) are expressed in terms of the function values, (12) takes the form

$$\sum_{j=0}^{k} a_j y_{n+1-j} = h^2 f_{n+1}. \quad (13)$$

The coefficients a_j are tabulated below.

Table 2. Coefficients a_j, $j=0(1)\,k, k=2(1)7$

k \ j	0	1	2	3	4	5	6	7
2	1	–2	1					
3	2	–5	4	–1				
4	$\frac{35}{12}$	$\frac{-104}{12}$	$\frac{114}{12}$	$\frac{-56}{12}$	$\frac{11}{12}$			
5	$\frac{45}{12}$	$\frac{-154}{12}$	$\frac{214}{12}$	$\frac{-156}{12}$	$\frac{61}{12}$	$\frac{-10}{12}$		
6	$\frac{812}{180}$	$\frac{-3132}{180}$	$\frac{5265}{180}$	$\frac{-5080}{180}$	$\frac{2970}{180}$	$\frac{-972}{180}$	$\frac{137}{180}$	
7	$\frac{938}{180}$	$\frac{-4014}{180}$	$\frac{7911}{180}$	$\frac{-9490}{180}$	$\frac{7380}{180}$	$\frac{-3618}{180}$	$\frac{1019}{180}$	$\frac{-126}{180}$

The coefficients a_j in a slightly different form are given in [4] for $k=2(1)6$. It can be seen that the local truncation error of the formula (13) is given by

$$L.T.E. = \delta_{0,k+1} h^{k+1} y^{(k+1)}(\eta) \tag{14}$$

It follows that the k-step method (13) has order $(k-1)$. For the method (13), we have

$$\rho(\xi) = \sum_{j=0}^{k} a_j \xi^{k-j} \quad \text{and} \quad \sigma(\xi) = \xi^k .$$

The roots of the characteristic equation $\rho(\xi) - \bar{h}\sigma(\xi) = 0$ of (13) tend to those of $\sigma(\xi) = 0$ which lie at the origin as $\bar{h} \to \infty$. The regions of absolute stability of (8) for $k=2(1)7$ are shown in Figures 1 to 6. (Taking real part on X-axis and imaginary part on Y-axis). The region of absolute stability is the region lying outside the boundary.

6. Explicit Methods. Putting $r=1$ in (8), we get a class of explicit methods given by

$$\sum_{m=0}^{k} \delta_{1,m} \nabla^m y_{n+1} = h^2 f_n . \tag{15}$$

From (11) it follows that $\delta_{1,m}$ is the coefficient of t^m in the expansion of

$(1-t)[\text{Log}\ (1-t)]^2$ in powers of t. The coefficients $\delta_{1,m}$ are tabulated below :

Table 3. Coefficient $\delta_{1,m}$ $m=0(1)$ 7

m	0	1	2	3	4	5	6	7
$\delta_{1,m}$	0	0	1	0	-1/12	-1/12	-13/180	-11/180

Differences in (15) are expressed in terms of function values, (15) takes the form

$$\sum_{j=0}^{k} \alpha_j y_{n+1-j} = h^2 f_n . \tag{16}$$

The coefficients α_j are tabulated below :

Table 4. Coefficients $\alpha_j : j=0(1)k,\ k=2(1)7$

k \ j	0	1	2	3	4	5	6	7
2	1	−2	1					
3	1	−2	0					
4	$\frac{11}{12}$	$\frac{-20}{12}$	$\frac{6}{12}$	$\frac{4}{12}$	$\frac{-1}{12}$			
5	$\frac{10}{12}$	$\frac{-15}{12}$	$\frac{-4}{12}$	$\frac{14}{12}$	$\frac{-6}{12}$	$\frac{1}{12}$		
6	$\frac{137}{180}$	$\frac{-147}{180}$	$\frac{-255}{180}$	$\frac{470}{180}$	$\frac{-285}{180}$	$\frac{93}{180}$	$\frac{-13}{180}$	
7	$\frac{126}{180}$	$\frac{-70}{180}$	$\frac{-486}{180}$	$\frac{855}{180}$	$\frac{-670}{180}$	$\frac{324}{180}$	$\frac{-90}{180}$	$\frac{11}{180}$

It can be seen that the local truncation error of the formula (16) is given by

$$L.T.E. = \delta_{1,k+1} h^{k+1} y^{(k+1)}(\eta). \tag{17}$$

It follows that the k-step method (17) has order $(k\text{–}1)$. When $k=2,3$ the method (17) reduces to the Stomer's method

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f_n, \tag{18}$$

which is absolutely stable for $h \in [-4,0]$. The regions of absolute stability for $k=4(1)7$ are shown in figures 7,8,9 and 10. (Taking real part on X–axis and imaginary part on Y-axis). The region of absolute stability is the region lying outside the boundary.

8. Conclusion. The methods based on numerical integration are found to have closed regions of absolute stability, the methods based on numerical Differentiation are found to be absolutely stable outside some closed boundaries.

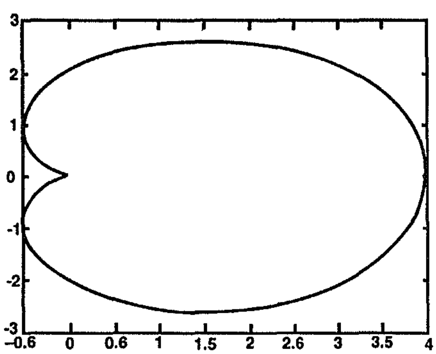

Fig.1 : $r=0$, $k=2$.

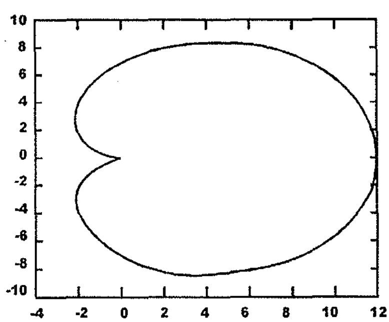

Fig.2 : $r=0$, $k=3$.

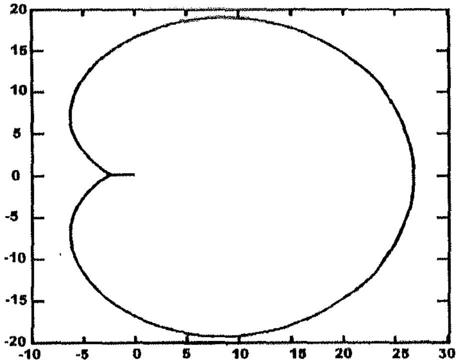

Fig.3 : r=0, k=4.

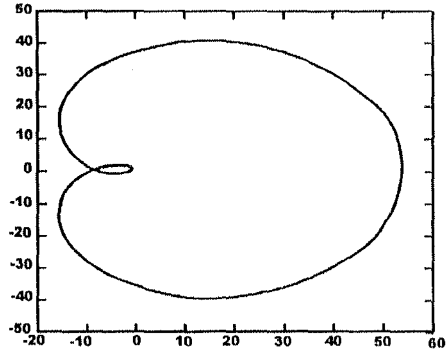

Fig.4 : r=0, k=5.

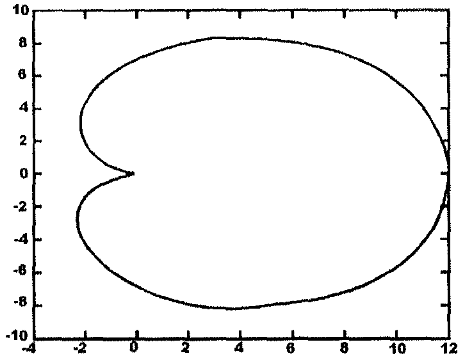

Fig.5 : r=0, k=6.

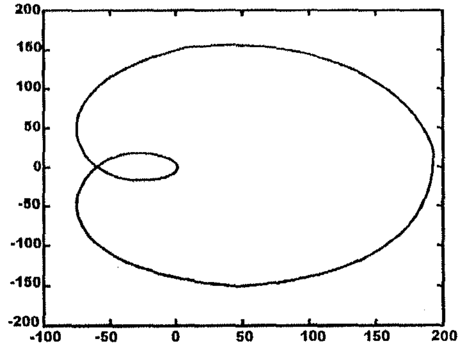

Fig.6 : r=0, k=7.

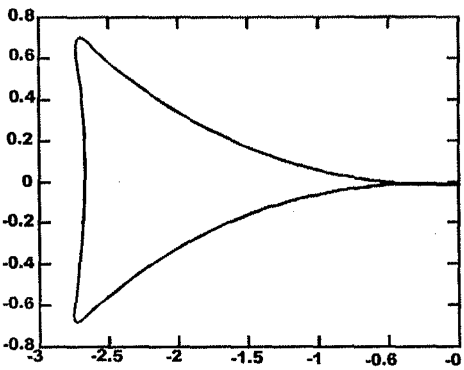

Fig.7 : r=1, k=4.

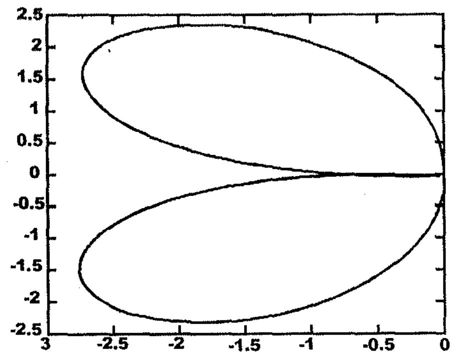

Fig.8 : r=1, k=5.

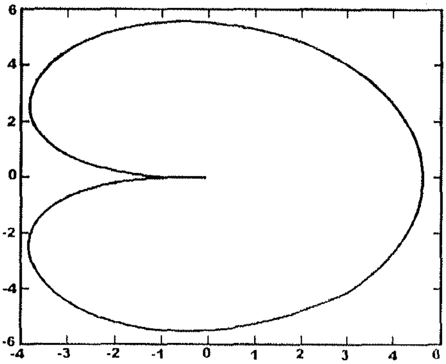

Fig.9 : r=1, k=6.

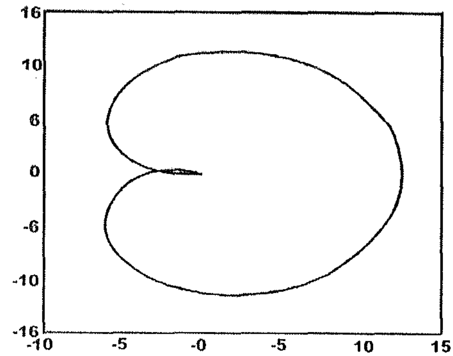

Fig.10 : r=1, k=7.

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