QUARTERLY TECHNICAL REPORT

for

October, November, December, 1965

Contract NAS 8-2559 (MI)

During the current quarter, the contract work has been done chiefly by Professor Wesson and Mr. John Edwards. As usual, Professor Shanks' participation has been reduced substantially because of administrative responsibilities.

However, work has continued on "error stabilizers" under the supervision of Professor Shanks. A great part of this work has been of a computational nature in order to get additional information on these stabilizers.

Professor Wesson has continued his investigation of predictor-corrector processes in the solution of differential equations. A method in which a new corrector is chosen each step has been developed for several orders, and has been tested for orders 3 and 5. The investigation included a close look at the roots of the characteristic equation.

Professor Wesson read a paper outlining his results at the November 12 meeting of the American Mathematical Society. The paper is submitted as part of this report.

FACILITY FORM 602
N66-16183 (ACCESSION NUMBER)
(THRU)
12 (PAGES)
1 (CODE)
CR 69882 (NASA CR OR TMX OR AD NUMBER)
19 (CATEGORY)

Respectfully submitted,

E. Baylis Shanks
Principal Investigator

cc: C. L. Bradshaw
Audie Anderson

GPO PRICE $ ______
CFSTI PRICE(S) $ ______
Hard copy (HC) $1.00
Microfiche (MF) .50
ff 653 July 65

A REPORT ON A PREDICTOR-CORRECTOR PROCESS IN WHICH THE SELECTION OF AN OPTIMUM CORRECTOR IS MADE EACH STEP •

By James R. Wesson, Vanderbilt University

1. Introduction. It is the purpose here to report the development and use of a predictor-corrector process in which a new corrector is selected at each step. The purpose of the program is to make a good compromise between truncation error and propagated error. The new process seems to be applicable to the numerical solution of a wide variety of differential equations.

We present in section 2 a one-parameter family of correctors, along with an examination of the characteristic roots. In section 3 we explain the method for choosing the optimum corrector from the fifth-order family. The program is sketched in section 4, and a comparison of the new method with other methods is given in section 5.

2. A family of stable correctors. The Adams corrector

$$y_{n+1} = y_n + h \sum_{i=0}^{n+1} B_i y_i' \tag{1}$$

is noted for its favorable stability properties. On the other hand the Newton-Cotes corrector

$$y_{n+1} = y_0 + h \sum_{i=0}^{n+1} C_i y_i' \tag{2}$$

• This work was done under NASA contract NAS8-2559.

has a smaller step error but is on the boundary of the set of stable correctors. For $h = 0$, the characteristic roots of (1) are $1,0,\ldots,0$ and the characteristic roots of (2) are the (n+1)-th roots of unity.

We now consider the one-parameter family of correctors obtained by multiplying equations (1) and (2) by r and $1 - r$ respectively, and then adding the results. As r varies from 1 to 0, the corrector changes from (1) to (2).

For $h = 0$ and $0 \leq r \leq 1$ it is easy to show that no characteristic root is outside the unit circle. For $-x^{n+1} + rx^n + (1-r) = 0$ and $x \neq 0$ give $|x| \leq r + (1-r)\,|x|^{-n}$. Then $|x| > 1$ is impossible. When $0 < r < 1$, every root except the single root 1 is within the unit circle. For any other root would satisfy $(1+a)x^n + x^{n-1} + x^{n-2} + \cdots + x + 1 = 0$, where $r/(1-r) = a > 0$. Then multiplying by $x - 1$ gives

$$x^{n+1} - 1 = -ax^n(x-1), \quad \text{and}$$

$$x^{-n-1} + ax^{-1} = 1 + a.$$

Suppose $|x| = 1$. Then $|x^{-n-1} + ax^{-1}| = |x^{-n} + a| = 1 + a$. The point x^{-n} is on the unit circle and also on the circle with center $-a$ and radius $1 + a$. Hence $x^n = 1$. But $x \neq 1$. Then $x^n = 1$ gives $x^{n-1} + x^{n-2} + \cdots + 1 = 0$, $(1+a)x^n = 0$, and $x = 0$, a contradiction.

3. Choice of a corrector. It is well known that the selection of the best corrector for solving $y' = f(x,y)$ with stepsize h depends on $K = h\,f_y$ [2, p.8; 3, p. 197; 4, p. 218]. Recall that each corrector of the family of section 2 is determined by r, and suppose we use K to determine $r = r(K)$. Then we may change the corrector as often as we take time to compute K and $r(K)$.

In this report, the function $r(K)$ has been determined empirically for fifth-order correctors. Note that equations of the form $y' = ay$ present a constant K. For such an equation various correctors (that is, various values of r) were tested and compared. The best one was used to determine $r(K)$. Other values of K were obtained by varying a in $y' = ay$, or by varying h. Each of these was used to determine another best value of r. A least squares smoothing gave the equation $r = 0.57K^2 - 1.18K + 0.18$ for $|K| \leq 0.5$. Then as K varies from -0.5 to 0 to 0.5, r varies from 0.91 to -0.27. The decision to permit r to get outside the interval $[0,1]$ is risky. However, the best results for the equations solved were obtained by using r as defined above.

4. <u>A sketch of the program</u>. The following process by Shanks [6, p. 19] is used to produce three starting points.

$$k_0 = hf(x_0, y_0)$$
$$k_1 = hf(x+h/300,\ y+k_0/300)$$
$$k_2 = hf(x+h/5,\ y+(1/5)(-29k_0+30k_1))$$
$$k_3 = hf(x+3h/5,\ y+(1/5)(323k_0-330k_1+10k_2))$$
$$k_4 = hf(x+14h/15,\ y+(1/810)(-510104k_0+521640k_1-12705k_2+1925k_3))$$
$$k_5 = hf(x+h,\ y+(1/77)(-417923k_0+427350k_1-10605k_2+1309k_3-54k_4))$$
$$y_1 = y_0+(1/3696)(198k_0+0k_1+1225k_2+1540k_3+810k_4-77k_5).$$

Then the predictor

$$y_4 = 10y_1 + 9y_2 - 18y_3 + h(3y_0' + 18y_1' + 9y_2')$$

gives y_4, and y_4' is predicted as $f(x_4, y_4)$. The corrector (take $r = 1$ initially)

$$y_4 = ry_3 + (1-r)y_0 + \frac{h}{720}\Big[(224 + 27r)y_4'$$

$$+ (1024 - 378r)y_3' + (384 - 648r)y_2' + (1024 - 918r)y_1'$$

$$+ (224 - 243r)y_0'\Big]$$

gives a corrected value of y_4, which leads to a corrected value of $y_4' = f(x_4, y_4)$, etc. (In the examples described here, the corrector is applied twice each step.)

Now we compute a new value of r for the next step. Take $K = h(\overline{y_4'} - y_4') / (\overline{y_4} - y_4)$, where $\overline{y_4'}$, $\overline{y_4}$ are predicted values, and y_4', y_4 are the last corrected values. Then compute $r = 0.57K^2 - 1.18K + 0.18$ if $K \leq 0.5$. In case $\overline{y_4} - y_4 = 0$, use $r = 1$. For $K \leq -0.5$ take r constant. Similarly for $k \geq 0.5$ take r constant.

5. Comparison with other methods. The following table indicates how the method formulated above competes with methods in which a fixed corrector (value of r) is used at each step. Each solution is started at $(0,1)$ with $h = 0.05$ and continued to $x = 10$. The programs are identical in every respect, except in the choice of r.

In the first six columns of the table r is fixed. The first column are the results for the Adams corrector $(r = 1)$. When $K > 0$, values of r close to 0 are used, and this gives a small truncation error with no apparent damage to the numerical stability of the process. For $K < 0$, r must be nearer to 1, or else the process becomes unstable. For all values of K the new process competes very well with any of the others. For $k < 0$ it is on a par with the best of the others, and for $k > 0$ it surpasses the others. It seems to be depend-

TABLE OF RELATIVE ERRORS AT $x = 10$

EQUATION	VALUE OF r: 1.0	0.8	0.6	0.4	0.2	0.0	New r Each Step
$y' = xy$	$.56 \times 10^{-2}$	$.37 \times 10^{-2}$	$.25 \times 10^{-2}$	$.16 \times 10^{-2}$	$.97 \times 10^{-3}$	$.45 \times 10^{-3}$	$.11 \times 10^{-4}$
$y' = -xy$	$.15 \times 10^{-1}$	$.39 \times 10^{-2}$	$.42 \times 10^{-1}$	$.33 \times 10^{7}$	---	---	$.49 \times 10^{-2}$
$y' = 5y \cos 5x$	$.72 \times 10^{-3}$	$.52 \times 10^{-3}$	$.31 \times 10^{-3}$	$.17 \times 10^{-3}$	$.10 \times 10^{-3}$	$.11 \times 10^{-4}$	$.68 \times 10^{-4}$
$y' = 10y \cos(x/2)$	$.31 \times 10^{-1}$	$.79 \times 10^{-2}$	$.35 \times 10^{-2}$	$.86 \times 10^{3}$	---	---	$.98 \times 10^{-2}$

able for a broad class of equations.

6. Conclusion. Changing the corrector each step is one way of automatically achieving a balance between numerical stability and truncation error. A new corrector each step can be selected without additional functional evaluations and with a relatively small increase in computing time. It is to be expected that the empirical formula for r (see section 3) can be improved. Indeed, the author has experimented with a number of different functions $r = r(K)$, but none have been appreciably superior to the one used.

APPENDIX

The derivation and treatment of formulas (1) and (2) of section 2 are well known for example, [1, p. 10 and 3, p. 157]. The remainder term for the fifth-order corrector given in section 4 is

$$-\frac{3rh^6f^{(6)}}{160} - \frac{8(1-r)h^7f^{(7)}}{945}.$$ For $r = 0$, the corrector is of order six.

Nashville, Tennessee
November, 1965

REFERENCES

1. Collatz, L. The numerical treatment of differential equations, 3rd edition, Springer, Berlin, 1960.

2. Dahlquist, Germund. Stability and error bounds in the numerical integration of ordinary differential equations, Almquist and Wiksells Boktrycheri AB, Uppsala, 1958.

3. Hamming, R. W. Numerical methods for scientists and engineers, McGraw-Hill, New York, 1962.

4. Henrici, Peter. Discrete variable methods in ordinary differential equations, Wiley, New York, 1962.

5. Milne, W. E. Numerical solution of differential equations, Wiley, New York, 1953.

6. Shanks, E. B. Higher order approximations of Runge-Kutta type, National Aeronautics and Space Administration Technical Note D-2920, Washington, D. C., 1965.