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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

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SUMMARY

One widely used technique for the numerical solution of a differential equation is to approximate the differential equation by a difference equation, and then to solve this difference equation. This paper treats the stability of the solutions obtained by this method. An original development leading to a definition of stability shows a relation between stability and certain properties of the systems of differential equations to be solved. Previous investigations (with the exception of Dahlquist's work) have shown a similar relation, but were limited to the consideration of a single equation. Dahlquist's theory, while valid for systems of equations, shows no such relation.

INTRODUCTION

A large part of the computer time at NASA Manned Spacecraft Center, Houston, Texas, is devoted to the numerical solution of differential equations. In order to reduce this computing time, it is necessary that accurate, more rapid methods of numerical integration be developed. One important criterion of accuracy in selecting a method is that it be stable. The stability of a method is that property which causes an error introduced at some step to tend to decay in succeeding steps, rather than to grow and eventually destroy the usefulness of the approximate solution. It is, therefore, extremely important that users of numerical integration procedures be familiar with the concept of stability. The purpose of this paper is to discuss stability of numerical methods, and to extend the definition of stability to systems of equations.

SYMBOLS

a constant

$F(x, Y)$, $Y(x)$ m-dimensional vector functions

$F_n = F(x_n, Y_n)$

$f(x, Y)$ component of F

$f_n = f\left(x_n, Y_n\right)$

h integration step-size

$x_n = a + nh$

Y_n an approximation to $Y\left(x_n\right)$

$y(x)$ component of Y

y_n an approximation to $y\left(x_n\right)$

$\epsilon_k = Y\left(x_k\right) - Y_k$

$\epsilon_k' = F\left[x_k, Y\left(x_k\right)\right] - F\left(x_k, Y_k\right)$

STABILITY AND CONVERGENCE

Consider the difference equation

$$a_k Y_{n+k} + a_{k-1} Y_{n+k-1} + \cdots + a_0 Y_n = h\left(b_k F_{n+k} + b_{k-1} F_{n+k-1} + \cdots + b_0 F_n\right) \quad (1)$$

to solve the ordinary differential equation

$$\left. \begin{aligned} Y' &= F(x, Y) \\ Y(a) &= Y_0 \end{aligned} \right\} \quad (2)$$

Let $Y(x)$ be the solution to equation (2), and define the operator

$$L\left[Y(x)\right] = \sum_{i=0}^{k} \left[a_i Y(x + ih) - h b_i Y'(x + ih)\right]$$

By expanding L in a power series about x, it can be shown that

$$L\left[Y(x)\right] = O\left(h^{p+1}\right)$$

if, and only if, the following p+1 linear relations hold:

Statement (a) $$\sum_{i=0}^{k} a_i = 0$$

Statement (b) $$\sum_{i=0}^{k} \left[a_i \frac{i^s}{s!} - b_i \frac{i^{s-1}}{(s-1)!} \right] = 0 \qquad (s = 2, \ldots, p)$$

Statement (c) $$\sum_{i=0}^{k} \left(a_i i - b_i \right) = 0 \qquad\qquad (s = 1)$$

Definition A.   Let p be the largest value of s for which statements (a) to (c) of the above assertion hold. Then p will be called the degree of the operator L or the degree of the difference equation (1).

Definition B.   The number of preceding points occurring, explicitly or implicitly, in equation (1) will be called the order of the operator L or the order of the difference equation (1).

(The above definitions are those used by Dahlquist (ref. 1). Some authors define the quantity of definition A as the order of the method and refer to the quantity in definition B as the step number of the method.)

As a simple example, consider the point-slope difference equation

$$Y_{n+1} - Y_n = hF_n$$

This method has order 1 since it uses only one preceding point Y_n to compute Y_{n+1}. The equation

$$L\left[Y(x) \right] = Y(x + h) - Y(x) - hY'(x)$$

is the operator associated with the difference equation. Statement (a) of definition A holds, since $a_1 = 1$ and $a_0 = -1$. The largest value of s for which statement (b) is true is determined in the following manner:

If s = 1, then

$$\sum_{i=0}^{1} a_i i - b_i = -1 + 1 = 0$$

and, if s = 2, then

$$\sum_{i=0}^{1} \frac{a_i}{2} i^2 - b_i i = \frac{a_i}{2} - b_1 = \frac{1}{2} \neq 0$$

Therefore, the point-slope formula has degree 1.

The polynominals

$$\rho(\xi) = a_k\xi^k + a_{k-1}\xi^{k-1} + \ldots + a_0$$

$$\sigma(\xi) = b_k\xi^k + b_{k-1}\xi^{k-1} + \ldots + b_0$$

(3)

can be associated with the difference equation (1), and hence, with every pair of polynomials of the type of equation (3), can be associated a difference equation of the form of equation (1), provided the degree of ρ is at least equal to the degree of σ. The following assumptions can be made concerning the polynomials of equation (3):

Assumption (a). The coefficients a_i, b_i ($i = 0, \ldots, k$) are real, $a_k \neq 0$.

Assumption (b). The polynomials $\rho(\xi)$ and $\sigma(\xi)$ have no common factor.

Assumption (c). The degree p of the operator L is at least 1.
(Condition of consistency)

Definition C. The difference equation (1) is said to be stable if the following assumptions are satisfied in addition to assumptions (a) to (c):

Assumption (d). The roots of $\rho(\xi)$ are located within or on the unit circle.

Assumption (e). The roots on the unit circle are distinct.

Theorem I. A necessary and sufficient condition for convergence of the linear multistep method of equation (1) is that the condition of stability is satisfied.

The proof of Theorem I and also the proofs of the following three theorems are given in references 1 and 2.

Theorem II. The degree p of a stable operator of order K can never exceed $K + 2$. If K is odd, the degree cannot exceed $K + 1$.

Theorem III. If an operator of even order K is stable, then the conditions

and

$$a_i = -a_{k-i}$$

$$b_i = b_{k-i}$$

(4)

are necessary and sufficient in order that it should be of maximum degree $K + 2$. All roots of $\rho(\xi)$ then have unit modulus.

Definition D. The formula of equation (1) is said to be open if $b_k = 0$, and closed if $b_k \neq 0$.

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Theorem IV. If the degree p is greater than the order K and the method is stable, then the difference equation must be closed.

Actually $b_k/a_k > 0$. It is possible to construct an open, stable operator of degree $p = K$, starting from any polynomial $\rho(\xi)$, and satisfying assumptions (a) to (e).

As an example of an unstable method, consider the difference equation

$$Y_{n+1} - 2Y_n + Y_{n-1} = F_1(h,x,Y) \tag{5}$$

to solve the initial value problem $Y' = 0$, $Y(0) = 0$.

The associated polynomial $\rho(\xi)$ has a multiple root at $\xi = 1$ and therefore violates the condition of stability. Assume that $Y_{-1} = Y_{-2} = 0$ are given exactly. Further, assume that an error is made in computing Y_0 and the result is $Y_0 = \epsilon \neq 0$. Using the formula of equation (5) and computing several values give the following results:

$$Y_1 = 2\epsilon$$

$$Y_2 = 3\epsilon$$

$$Y_3 = 4\epsilon$$
$$\vdots$$
$$Y_n = (n + 1)\epsilon$$

It is then seen that in an unstable method, any error introduced can continue to grow in succeeding calculations until the approximate solution becomes worthless. A stable method does not allow growth of this type. For example, consider the point-slope formula

$$Y_{n+1} - Y_n = hF_n \tag{6}$$

and the more complicated formula

$$Y_{n+1} - \frac{1}{2}Y_n - \frac{1}{2}Y_{n-1} = F_2(h,x,Y) \tag{7}$$

The associated polynomials of equations (6) and (7) are respectively,

$$\rho - 1 = 0 \tag{8}$$

and
$$\rho^2 - \frac{1}{2}\rho - \frac{1}{2} = 0 \tag{9}$$

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The root of equation (8) is $\rho = 1$ and the roots of equation (9) are $\rho = 1$ and $\rho = -\frac{1}{2}$. Using equation (6) to solve the same problem as in the preceding example, it can be seen that the error in each step, after the error was introduced in the computation of Y_0, has the same magnitude as the error in Y_0. Using equation (7), a few values are computed:

$$Y_1 = \frac{\epsilon}{2}$$

$$Y_2 = \frac{3\epsilon}{4}$$

$$Y_3 = \frac{5\epsilon}{8}$$

$$\cdot$$
$$\cdot$$
$$\cdot$$

Notice that, assuming no further error is made, the error in step n is less than the error made in computing Y_0.

As Theorem I states, the condition of definition C is necessary and sufficient for convergence.

WEAK INSTABILITY

The second type of instability may allow unfavorable error growth in the immediate vicinity of zero step-size. Methods in which this can happen are called weakly or conditionally stable. This section is concerned with the integration of the single first-order equation

$$y' = f(x,y) \tag{10}$$

using the difference equation (1).

Define ϵ_k by the equation

$$\epsilon_k = y\left(x_k\right) - y_k$$

and ϵ_k' by the equation

$$\epsilon_k' = f\left[x_k, y\left(x_k\right)\right] - f_k$$

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It can be assumed that h is sufficiently small that, given a point x_k, $\frac{\partial f}{\partial y}$ is constant in the interval with end points $y(x_k)$ and y_k. Then, by the mean value theorem

$$\epsilon_k' = \frac{\partial f}{\partial y}\,\epsilon_k \tag{11}$$

By substituting the true values into equation (1), and then the computed values, and subtracting the two, the following difference equation is obtained for the error ϵ which was committed because the computed values were used rather than the true values.

$$a_k \epsilon_{n+k} + a_{k-1}\epsilon_{n+k-1} + \ldots + a_0 \epsilon_n = h\left(b_k \epsilon_{n+k}' + b_{k-1}\epsilon_{n+k-1}' + \ldots + b_0 \epsilon_n'\right) \tag{12}$$

On using equation (11) and defining $\bar{h} = \frac{\partial f}{\partial y}\,h$, equation (12) can be written as

$$\left(a_k - \bar{h}b_k\right)\epsilon_{n+k} + \left(a_{k-1} - \bar{h}b_{k-1}\right)\epsilon_{n+k-1} + \ldots + \left(a_0 - \bar{h}b_0\right)\epsilon_n = 0 \tag{13}$$

Now

$$\epsilon_n = c_1 \rho^n + c_2 \rho_2^{\,n} + \ldots + c_k \rho_k^{\,n} \tag{14}$$

where the $\rho_i, i = 1, \ldots, k$ are the roots of the associated polynominal

$$\left(a_k - \bar{h}b_k\right)\rho^k + \left(a_{k-1} - \bar{h}b_{k-1}\right)\rho^{k-1} + \ldots + \left(a_0 - \bar{h}b_0\right) = 0 \tag{15}$$

It should be noted that if the roots of equation (15) are not simple, the form of the previous equation for ϵ_n (eq. (14)) will be slightly different. As an example, if ρ_1 is a root of multiplicity 2,

$$\epsilon_n = \left(c_1 + c_2 n\right)\rho_1^{\,n} + c_3 \rho_3^{\,n} + \ldots + c_k \rho_k^{\,n}$$

Relative stability can now be defined as follows:

Definition E. In the region $\bar{h} < = 0$, the difference equation (1) is said to be stable if the roots of the polynomial of equation (15) are contained within the unit circle. Note that when $\bar{h}$ is positive, or $\frac{\partial f}{\partial y}$ is positive, the error already grows exponentially from the nature of the error equation (11). This growth is not regarded as instability in the method.

The following theorem from reference 3 gives a stability criterion for a difference equation.

Theorem V. The difference equation (1) is stable if, and only if, the matrix

$$A_{r,s} = \sum_{i=0}^{\min(r,s)} \left(c_{k+i-r} c_{k+i-s} - c_{r-i} c_{s-i} \right)$$

$$(r,s = 0,1, \ldots , k - 1)$$

is positive definite, where

$$c_j = a_j - \bar{h} b_j \qquad\qquad (j = 0,1, \ldots , k)$$

Reference 4 shows that the square matrix $A_{r,s}$ of the above theorem is symmetric about both diagonals, that is,

$$A_{r,s} = A_{s,r}$$

and

$$A_{r,s} = A_{k-s-1, \ k-r-1}$$

Thus, the number of computations involved in the application of Theorem V to a difference equation is reduced considerably.

References 5 and 6 use the fact that the roots of a polynomial are continuous functions of the coefficients of the polynomial to study stability of integration formulas. This property of roots of polynomials is proven in reference 7. It is possible to vary $\bar{h}$ in equation (15) and plot the roots as a function of $\bar{h}$ to determine the region of stability of equation (1).

It is thought that the method of Theorem V is more precise than the aforemention method; however, computing the characteristic roots of $A_{r,s}$ might not be simple. The previous method, while not quite as precise, should give a satisfactory bound on $\bar{h}$.

It is shown in reference 8 that if a predictor-corrector method is used where the corrector formula is used only once per integration step, the stability of the method is dependent on the predictor formula as well as on the corrector. Therefore, in arriving at equation (15), an error equation must be derived for the predicted value, and this value must be substituted into the error equation for the corrected value.

Finally, it should be noted that this latter concept of stability has not been extended to a system of differential equations.

EXTENSION OF THE DEFINITION OF STABILITY

Let $Z_j = Y(x_j) - Y_j$ and $Z_j' = F\left[x_j, Y(x_j)\right] - F_j$. Substituting $Y(x_j)$ and Y_j into equation (1), and subtracting in the same manner as in the preceding section, yield the following difference equation for the error Z,

$$a_k Z_{n+k} + \ldots + a_0 Z_n = h\left(b_k Z_{n+k}' + \ldots + b_0 Z_n'\right) \tag{16}$$

Let

$$A = a_{ij}$$

where $a_{ij} = \dfrac{\partial f_i}{\partial y_j}$, the terms f_i and y_j being the ith and jth components of the vectors F and Y, respectively. The assumption is now made that a_{ij} is constant and it follows immediately from the mean value theorem that

$$Z_j' = A Z_j \tag{17}$$

Upon substituting equation (17) into equation (16), the following difference equation is obtained

$$a_k Z_{n+k} + \ldots + a_0 Z_n = hA\left(b_k Z_{n+k} + \ldots + b_0 Z_n\right) \tag{18}$$

For purposes of simplification, the following theorem is used.

Theorem VI. Every complex $n \times n$ matrix A is similar to a matrix of the form

$$J = \begin{pmatrix} J_0 & 0 & 0 & . & . & . & 0 \\ 0 & J_1 & 0 & . & . & . & 0 \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & . & J_s \end{pmatrix} \tag{19}$$

where J_0 is a diagonal matrix with diagonal $\lambda_1, \lambda_2, \ldots, \lambda_q,$ and

$$J_i = \begin{pmatrix} \lambda_{q+i} & 1 & 0 & 0 & . & . & . & 0 & 0 \\ 0 & \lambda_{q+i} & 1 & 0 & . & . & . & . & . \\ . & . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & . & . & . & \lambda_{q+i} & 1 \\ 0 & 0 & 0 & 0 & . & . & . & 0 & \lambda_{q+i} \end{pmatrix}$$

$$(i = 1, \ldots, s)$$

The λ_j, $j = 1, 2, \ldots, q + s$ are the characteristic roots of A and need not all be distinct. If the λ_j are all simple, then A is similar to a diagonal matrix whose diagonal elements are the characteristic roots of A. (For a proof, reference could be made to ref. 9 or almost any of the numerous texts on linear algebra and matrix theory.) The form of equation (19) is noted by $J(A)$.

By the preceding theorem, there exists a non-singular matrix P, such that $PAP^{-1} = J(A)$. Set $\epsilon = PZ$, solve for $Z = P^{-1}\epsilon$, and substitute into equation (18) to obtain

$$a_k \epsilon_{n+k} + \ldots + a_0 \epsilon_n = h\, J(A)\left(b_k \epsilon_{n+k} + \ldots + b_0 \epsilon_n\right) \qquad (20)$$

Transforming equation (17) in a similar manner, the following equation is obtained:

$$\epsilon' = J(A)\epsilon \qquad (21)$$

Only those error components of equation (21) which involve characteristic roots of A with negative real parts are considered, since the error in the other components already grow exponentially. This error growth due to the nature of the error equation (21) is not regarded as instability of the method.

Let

$$a_k \epsilon_{j,n+k} + \ldots + a_0 \epsilon_{j,n} = h\lambda_j\left(b_k \epsilon_{j,n+k} + \ldots + b_0 \epsilon_{j,n}\right)$$

$$+ hc\left(b_k \epsilon_{j+1,n+k} + \ldots + b_0 \epsilon_{j+1,n}\right) \qquad (22)$$

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be an arbitrary equation from the system of equations (20) where λ_j has negative real parts. Note that c is either 0 or 1. If c is 0, only the roots of the following characteristic polynomial

$$\left(a_k - h\lambda_j b_k\right) x^k + \ldots + \left(a_0 - h\lambda_j b_0\right) = 0 \tag{23}$$

need to be proved to lie within the unit circle.

For the case $c = 1$, the following theorem will be needed.

Lemma I. Let $f(E) = a_0 + a_1 E + \ldots + a_k E^k$ be a polynomial with root $R \neq 0$. There exists an integer $j \leq k$ such that

$$\sum_{i=0}^{k} a_i i^j R^i \neq 0$$

Proof. Consider the $K + 1$ homogeneous equations in $k + 1$ unknowns

$$\left.\begin{aligned}
x_0 + Rx_1 + R^2 x_2 + \ldots + R^k x_k &= 0 \\
Rx_1 + 2R^2 x_2 + \ldots + kR^k x_k &= 0 \\
\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \\
Rx_1 + 2^k R^2 x_2 + \ldots + k^k R^k x_k &= 0
\end{aligned}\right\} \tag{24}$$

The determinant of the matrix of coefficients of equation (24) reduces to the determinant

$$\begin{vmatrix}
R & 2R^2 & \ldots & kR^k \\
R & 2^2 R^2 & \ldots & k^2 R^k \\
\cdot & \cdot & \ldots & \cdot \\
R & 2^k R^2 & \ldots & k^k R^k
\end{vmatrix}$$

Factoring iR^i out of the ith column of equation (25) and using the property that $|A| = |A^T|$ for any square matrix A, equation (25) becomes

$$C \begin{vmatrix} 1 & 1 & . & . & . & 1 \\ 1 & 2 & . & . & . & 2^{k-1} \\ . & . & . & . & . & . \\ 1 & k & . & . & . & k^{k-1} \end{vmatrix} = C(-1)^k \prod_{1 \le i \le j \le k} (i - j) \ne 0 \qquad (26)$$

Since the determinant of the matrix of coefficients is non-zero, equation (24) can have only the trivial solution and therefore the coefficients of $f(E)$ cannot be a solution.

Theorem VII. Let E be an operator defined by

$$Ey_n = y_{n+1}$$

and let

$$f(E)y_n = An^r R^n \qquad (27)$$

be a non-homogeneous difference equation where $R \ne 0$ is a root of $f(E) = a_0 + a_1 E + . . . + a_k E^k$. Then, there exists an integer j, and $r + 1$ numbers, $B_j, B_{j+1}, . . . , B_{j+r}$, so that

$$y_n^P = \sum_{i=0}^{r} B_{j+i} n^{j+i} R^n \qquad (28)$$

is a particular solution to equation (27).

Proof. By Lemma I, there exists an integer j, so that

$$\sum_{i=0}^{k} a_i i^j R^i \ne 0$$

Assume that j is the minimum such integer and that y_n^P has the form of equation (28).

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Then

$$f(E)y_n^P = R^n \sum_{i=0}^{k} a_i R^i \left[B_j (n + i)^j + B_{j+1}(n + i)^{j+1} + \ldots + B_{j+r}(n + i)^{j+r} \right] \tag{29}$$

Equating coefficients of n^i, $i = 0, \ldots, r$, yields the following $r + 1$ linear equations in $r + 1$ unknowns:

$$\left. \begin{array}{l} \left(\sum\limits_{i=0}^{k} a_i i^j R^i \right) B_j + \left(\sum\limits_{i=0}^{k} a_i i^{j+1} R^i \right) B_{j+1} + \ldots + \left(\sum\limits_{i=0}^{k} a_i i^{j+r} R^i \right) B_{j+r} = 0 \\[2em] \left[\binom{j+1}{j} \sum\limits_{i=0}^{k} a_i i^j R^i \right] B_{j+1} + \ldots + \left[\binom{j+r}{j+r-1} \sum\limits_{i=0}^{k} a_i i^{j+r-1} R^i \right] B_{j+r} = 0 \\[2em] \cdots \cdots \\[1em] \left[\binom{j+r}{j} \sum\limits_{i=0}^{k} a_i i^j R^i \right] B_{j+r} = A \end{array} \right\} \tag{30}$$

The coefficients of n^i for $i > r$ are identically zero. For considering the coefficient of n^{r+m}, $1 \le m \le j$,

$$\sum_{i=0}^{k} a_i R^i B_{r+m} + \binom{r+m+1}{1} \sum_{i=0}^{k} a_i i R^i B_{r+m+1} + \ldots + \binom{r+j}{j-m} \sum_{i=0}^{k} a_i i^{j-m} R^i B_{r+j}$$

Each B has a coefficient with a factor $\sum\limits_{i=0}^{k} a_i i^m R^i$ where $m < j$. Therefore the coefficient of each B is zero.

Now consider again the non-homogeneous system of equations (30). It obviously has a solution, since its matrix of coefficients is triangular with all non-zero diagonal elements. Therefore, the $r + 1$ numbers $B_j, B_{j+1}, \ldots, B_{j+r}$ exist and the Theorem is proved.

Let E be the operator defined in Theorem VII. That is,

$$E\epsilon_{i,n} = \epsilon_{i,n+1}$$

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and

$$f(E) = \left(a_k - h\lambda_j b_k\right)E^k + \left(a_{k-1} - h\lambda_j b_{k-1}\right)E^{k-1} + \ldots + \left(a_0 - h\lambda_j b_0\right) \tag{31}$$

where the a_i and b_i, $i = 1, \ldots, k$, are defined by equation (1).

Consider now equation (22) where $c = 1$. There exists some positive integer r such that

$$\lambda_{j+r} = \lambda_{j+r-1} = \ldots = \lambda_j$$

and

$$f(E)\epsilon_{j+r,n} = 0 \tag{32}$$

Assume further that r is the least such integer. Therefore,

$$\epsilon_{j+r,n} = \sum_{s=1}^{m} \sum_{i=1}^{j_s} A_i n^{i-1} x_s^n \tag{33}$$

where x_i is a root of equation (23) of multiplicity j_i, $i = 1, \ldots, m$.

Substituting equation (33) into the equation for ϵ_{j+r-1} the following non-homogeneous difference equation is obtained:

$$f(E)\epsilon_{j+r-1,n} = \sum_{s=1}^{m} \sum_{i=1}^{j_s} B_i n^{i-1} x_s^n \tag{34}$$

Therefore, for some integer p

$$\epsilon_{j+r-1,n} = \sum_{s=1}^{m} \sum_{i=0}^{p} c_i n^i x_s^n \tag{35}$$

since the particular solution is of this form by Theorem VII and the solution of the homogeneous equation has the same form as equation (33). Hence, by induction, there exists an integer q such that

$$\epsilon_{j,n} = \sum_{s=1}^{m} \sum_{i=0}^{q} D_i n^i x_s^n \tag{36}$$

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Therefore, if $|x_s| < 1$, $s = 1, \ldots, m$, the error vector ϵ in the transformed equations decreases to O as n increases and hence the error vector Z also converges to O. Stability is now defined as follows:

Definition F. Let λ_j, $j = 1, \ldots, m$, denote the characteristic roots of $A = (a_{ij})$, $a_{ij} = \dfrac{\partial f_i}{\partial y_j}$. The difference equation (1) is stable if, for all λ_j with negative real parts, the roots of

$$\left(a_k - h\lambda_j b_k\right) x^k + \ldots + \left(a_0 - h\lambda_j b_0\right) = 0 \tag{37}$$

lie within the unit circle.

CONCLUSIONS

It has been shown that the region of stability of a method, if one exists, is dependent on the characteristic roots of the matrix A. If this information is available, it is possible to determine the step-size to insure that calculations are within this stability region. If, however, there is interest only in the existence of a stability region, this can be guaranteed by requiring that all the roots of the associated polynomial, with the exception of the principal root, lie within the unit circle.

Manned Spacecraft Center
    National Aeronautics and Space Administration
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