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A Computer Program for Determining Truncation Error Coefficients for Runge-Kutta Methods

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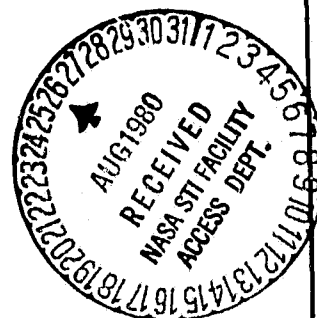
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National Aeronautics and
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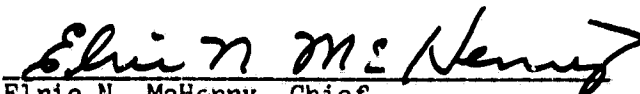
SHUTTLE PROGRAM

A COMPUTER PROGRAM FOR DETERMINING
TRUNCATION ERROR COEFFICIENTS
FOR RUNGE-KUTTA METHODS

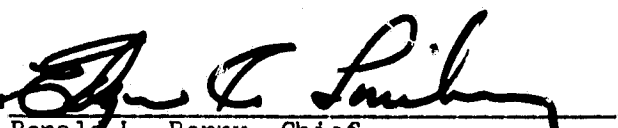
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1.0 INTRODUCTION

The solution of the initial value problem for ordinary differential equations (ODE's)

$$\frac{dy}{dt} = f(t,y), \quad y(t_0) = y_0 \quad (1)$$

may be treated by several different numerical methods. Runge-Kutta (RK) algorithms are a type of method well suited to solving equation (1) for many classes of functions, f , because of their simplicity and their accuracy. The RK algorithm is derived using a direct comparison with a truncated Taylor series, giving the accuracy of the Taylor series without the difficulty of determining complicated partial derivatives. The comparison between the Taylor series expansion of the solution vector and the solution determined by the RK algorithm results in a number of expressions referred to as truncation error coefficients, $T_{i,j}$. Associated with each term of order i in the Taylor series (or with each power of h , the integration stepsize) are λ_i truncation error coefficients. For an RK algorithm to be of order p , the $T_{i,j}$ coefficients must be identically zero for $i = 1, \dots, p$; $j = 1, \dots, \lambda_i$. These vanishing truncation error coefficients are referred to as equations of condition. The nonvanishing error coefficients, however, are of equally great importance since they indicate how closely the RK solution approximates a Taylor series solution of higher order. The equations of condition determine the validity of an RK algorithm; the nonvanishing error coefficients explain the differences between particular RK algorithms of the same order. While a user may apply an RK algorithm, never considering the truncation error coefficients, awareness of the effect of these terms is important both in the selection of a specific algorithm and in the analysis of difficulties encountered during the solution of a particular ODE.

D. G. Bettis,^a has developed an algorithm for generating the truncation error coefficients for RK methods designed to treat systems of both first- and second-order ODE's directly. The recursive nature of this algorithm lends itself readily to computer programming, generating high order error coefficients with little added difficulty. Such an algorithm, implemented in a numerical code, is an essential tool for anyone developing coefficients for RK algorithms and is of interest to the user of RK methods in analyzing the effectiveness of specific RK algorithms. A Fortran subroutine, RKEQN, written to accompany reference 1, generated the truncation error coefficients through order 10 but required a great amount of storage location, particularly when a double precision version of the program was needed. The basic structure of this original program has been reformulated to reduce storage requirements significantly and to accommodate variable dimensioning. This new Fortran program, SUBROUTINE RKEQ, determines truncation error coefficients for RK algorithms in the sequence presented in reference 1 for orders 1 through 10 and extends the order of coefficients

^aFrom a private communication with D. G. Bettis, 1978.

through 12 with the 11th- and 12th-order terms determined following the patterns used to establish the lower order coefficients. Both subroutines (RKEQN and RKEQ) are also written to treat RK m-fold methods (refs. 2 and 3) which utilize m known derivatives of f to increase the order of the algorithm. Setting m = 0 gives the classical RK algorithm.

2.0 THE GENERATION OF TRUNCATION ERROR COEFFICIENTS

The solution of equation (1) at $t_1 = t_0 + h$, using the RK algorithm, is written

$$y_1 = y_0 + \sum_{k=0}^p c_k f_k \quad (2)$$

where

$$f_0 = f(t_0, y_0)$$

$$f_k = f(t_0 + \alpha_k h, y_0 + h \sum_{\lambda=0}^{k-1} \beta_{k,\lambda} f_\lambda)$$

where $p + 1$, the number of evaluations of f computed, is referred to as the number of stages. The truncation error coefficients, $T_{i,j}$, determined by comparing the Taylor series expansion of equation (2) with the Taylor series expansion of the solution about t_0 , are nonlinear combinations of the C , α , and β coefficients. For the classical RK algorithm, the j th error coefficient of order i assumes the form

$$T_{i,j} = \{F_{i,j} - 1/(pA_{i,j})\} / B_{i,j} \quad (3)$$

$j = 1, \dots, \lambda_i$ where $p = i$. For the m -fold algorithm, $p = m + 1$ and corresponds to the order of the term. (For $m = 0$, the m -fold algorithm is identical to the classical RK formula.) The $A_{i,j}$ and $B_{i,j}$ terms are constants (or functions of m for m -fold methods) and may be determined by recursive relations. (One should note that while references to m -fold RK algorithms may appear to complicate matters, the inclusion of these methods in RKEQ (or RKEQN) involves the insertion of only a few additional lines of coding. Once these additions are made, the classical RK error coefficients and the m -fold error coefficients are determined identically.) The complicated expression to generate in equation (3) is the $F_{i,j}$ term, which is a combination of the C , α , and β coefficients

$$F_{i,j} = \sum_{k=k_0}^p c_k S_{i,j,k} \quad (4)$$

with $S_{i,j,k}$ being a combination of α and β coefficients and where k_0 depends upon the number of summations embedded in $S_{i,j,k}$.

The algorithm developed by Bettis and used for generating these $S_{i,j,k}$, $A_{i,j}$, and $B_{i,j}$ terms is documented in reference 1, where the $S_{i,j,k}$ terms are written in an abbreviated notation, e.g., $S_{8,13} = \alpha^2\beta\alpha\beta\beta\alpha$, with the subscripting and embedded summations being suppressed. The rules for writing the entire $S_{i,j,k}$ terms are also described thoroughly in reference 1. For the sake of interpreting the program, however, a few features need to be known about generating the terms in abbreviated notation. Denoting the number of truncation error coefficients of order μ , by λ_μ , and suppressing the k subscript, the first $2\lambda_{\mu-1}$ $S_{i,j,k}$ expressions are generated from the $S_{i-1,j,k}$ terms. The remaining $\lambda_\mu - 2\lambda_{\mu-1}$ expressions, referred to as composite sums, are formulated as products of lower order S terms. The $A_{i,j}$ and $B_{i,j}$ constants are also generated from simple relationships involving previous A and B terms. In generating the first λ_{i-1} terms of order i , the $S_{i-1,j}$ expressions are premultiplied by an α . (Adjacent α 's represent actual multiplication.) Thus, $S_{9,13} = \alpha S_{8,13}$, $S_{13} = \alpha^3\beta\alpha\beta\beta\alpha$. The next λ_{i-1} terms, $S_{i,j}$, $j = \lambda_{i-1} + 1, \dots, 2\lambda_{i-1}$ are generated by premultiplying the $S_{i-1,j-\lambda_{i-1}}$ expressions by a β , e.g., $S_{9,128} = \beta S_{8,13} = \beta\alpha^2\beta\alpha\beta\beta\alpha$. (Adjacent β 's do not represent multiplication of the β coefficients since a summation sign precedes each β when the entire S term is written, e.g.,

$$S_{6,4,k} = \alpha^2\beta\beta\alpha = \alpha k^2 \sum_{\ell=2}^{k-1} \beta_{k,\ell} \sum_{m=1}^{\ell-1} \beta_{\ell,m} \alpha^m \quad (5)$$

($S_{6,4,k} \neq \alpha^2\beta^2\alpha$.) The recursion relations, then, for the first λ_{i-1} terms of order i , ($i > 2$), are

$$S_{i,j} = \alpha S_{i-1,j}$$

$$A_{i,j} = A_{i-1,j}$$

$$B_{i,j} = \mu B_{i-1,j}$$

for $j = 1, 2, \dots, \lambda_{i-1}$, where μ is the power of the leading α in the $S_{i-1,j}$ term, and

$$S_{i,j} = \beta S_{i-1,j-\lambda_{i-1}}$$

$$A_{i,j} = (m+i-1) A_{i-1,j-\lambda_{i-1}}$$

$$B_{i,j} = B_{i-1,j-\lambda_{i-1}}$$

for $j = \lambda_{i-1} + 1, \dots, 2\lambda_{i-1}$. ($S_{1,1} = 1$, and $S_{2,1} = \alpha$.) The first λ_{i-1} S expressions are referred to as alpha terms in subroutine RKEQ, while the next λ_{i-1} expressions are called beta terms. The remaining terms, composite sums, are generated by considering the weight factors of the S terms. The $S_{\mu,j}$ expressions have a weight factor of $\mu-1$ (i.e., the number of α and β coefficients included in the S term). The composite sums of order i are all products of $S_{\mu,j}$ terms having initial β coefficients, whose weight factors add up to $i-1$. Subroutine RKEQ determines these composite sums in a separate block of the subprogram, calling subroutine CROSS to perform the multiplication of the S, A, and B terms. The $A_{i,j}$ and $B_{i,j}$ terms of a composite sum are the products of the A and B constants whose corresponding S terms form the composite sum. (When an S term is raised to the power k , an additional $k!$ multiplies the B constant.)

3.0 DESCRIPTION OF THE FORTRAN PROGRAM

Subroutine RKEQ determines the truncation error coefficients (TEC) for a given set of RK coefficients and returns TERROR,

$$\text{TERROR} = \left\{ \sum_{j=1}^{\lambda_1} T_{1,j}^2 \right\}^{1/2}$$

for a specified order i . Since RK algorithms with embedded pairs of solutions, e.g. RK-Fehlberg formulas, are often studied, RKEQ is written to treat two algorithms simultaneously, which use identical α and β coefficients but

different C_k and \hat{C}_k coefficients. (TERROR is formed using the \hat{C}_k coefficients.) The Greek letters α_i and β_i are replaced by A(I) and B(I) and the $A_{i,j}$ and $B_{i,j}$ constants are denoted AA(I,J) and BB(I,J), respectively.

The input parameters for RKEQ are:

(1) The RK coefficients

- (a) A(K) α_k , the alpha coefficients
- (b) CO, C(K) C_0, C_k , the C_k coefficients for the first solution
- (c) CHO, CH(K) \hat{C}_0, \hat{C}_k , the \hat{C}_k coefficients for the second solution used to form TERROR
- (d) BO(K), B(K,L) $\beta_{k,0}, \beta_{k,l}$, the beta coefficients

where $K = 1, 2, \dots, R$, $L = 1, 2, \dots, K - 1$, R an integer with $R + 1$ being the number of stages of the algorithm, and

(2) The integers controlling orders and options

- (a) R = the index for dimensioning the RK coefficients
- (b) IORDER = the maximum order to be treated
- (c) ITERR = the order of TEC used to form TERROR
- (d) IOPT = the options for operating the program. For IOPT = 1, RKEQ computes and prints all TEC(I,J) for $I = 1, \dots, \text{IORDER}$. For IOPT = 2, RKEQ computes and prints TEC(IORDER, J) only. For IOPT = 3, RKEQ computes but does not print TEC(ITERR, J). (For all options TERROR is computed, which may require internal adjustments to the order.)
- (e) MFOLD = an integer giving the number of known derivatives of f . For the classical RK algorithm, MFOLD = 0.

(f) LS = a dimensioning index for the work arrays, S, AA and BB.

The output parameter for RKEQ is TERROR, the Euclidean norm of the TEC of order ITERR. Depending upon the option used, RKEQ may print values of TEC, but these are not returned to the main program.

Parameters S, AA, and BB are used internally by RKEQ to compute the TEC terms. To take advantage of variable dimensioning, these parameters are given in the calling sequence with dimensions S(LS,R), AA(LS), BB(LS). The RK coefficients should be dimensioned A(R), C(R), CH(R), B(R, R), BO(R), R an integer, where $R + 1$ is the number of stages for the algorithm.

The calling sequence for RKEQ is

```
SUBROUTINE RKEQ(A, C, CO, CH, CHO, B, BO, R, IORDER, ITERR, IOPT, MFOLD,
TERROR, S, LS, AA, BB).
```

which, if a printing option is used, will give the TEC from the C solution in the first column and the TEC from the CH solution in the second column. Integers IORDER, ITERR, and IOPT are reset within the subroutine, and any adjustments made to protect against exceeding dimension or option limits are made to the new variables, so that the user may enter constant values in the calling sequence of the driving program.

A sample calling sequence for a six-stage, fifth-order algorithm is

```
CALL RKEQ(A, C, CO, CH, CHO, B, BO, 5, 7, 6, 1, 0, TERROR, S, 48, AA, BB)
```

which computes and prints all TEC through order 7 for the classical RK formulas, using the 6th-order terms of the CH solution to form TERROR. Using the calling sequence

```
CALL RKEQ(A, CH, CHO, C, CO, B, BO, 5, 7, 6, 1, 0, TERROR, S, 48, AA, BB)
```

generates similar information except that TERROR is formed by the C solution

(and the \hat{C} TEC terms are now printed in the first column.)

The minimum value of LS for a given ORDER, I, is found in table I. A listing of subroutines RKEQ and CROSS may be found in the appendix.

TABLE I.- DIMENSIONING PARAMETER, LS, FOR ORDERS 1 THROUGH 12

ORDER	1	2	3	4	5	6	7	8	9	10	11	12
LSMIN	1	1	2	4	9	20	48	115	286	719	1842	4766

4.0 CONCLUDING REMARKS

A program, which evaluates the truncation error coefficients, is an essential tool in the development of Runge-Kutta algorithms and in the comparison of existing RK algorithms. By structuring the routine in the given form, a substantial savings in storage occurs in generating these truncation error coefficients using the recursive formulation presented by D. G. Bettis (ref. 1). The extension to orders higher than 12 is relatively simple but not of great practical use at the present time.

REFERENCES

1. Bettis, D. G.; and Horn, M. K.: Computation of Truncation Error Terms for Runge-Kutta Methods. TICOM Report 77-14, December 1977.
2. Fehlberg, E.: New High-Order Runge-Kutta Formulas with Step-size Control for Systems of First- and Second-Order Differential Equations. ZAMM, Vol. 44, 1964.
3. Fehlberg, E.: New High-Order Runge-Kutta Formulas with an Arbitrarily Small Truncation Error. ZAMM, Vol. 6, 1966.

APPENDIX A
SUBROUTINE RKEQ

	SUBROUTINE RKEQ(A,C,CO,CH,CHO,B,BO,R,	
1	IORDER,ITERR,IOPT,MFOLD,TERROR,S,LS,AA,BB)	00000200
	INTEGER R,ORDER,OPTION	00000300
	DOUBLE PRECISION A(R),C(R),CH(R),B(R,R),BO(R)	00000400
	DOUBLE PRECISION CO CHO	00000500
	DOUBLE PRECISION S(LS,R),AA(LS),BB(LS)	00000600
	DOUBLE PRECISION SUM1,SUM3,X1,ZERO,UNITY,TWO,	00000700
1	MP(12),MM(12),FACT(12)	00000800
	DOUBLE PRECISION P,PP1,PM1,PM2,ZAPP,TERROR	00000900
	DIMENSION M(12),LIMIT(12),INDEX(11)	00001000
	LOGICAL EVEN	00001100
C		00001200
	DATA LIMIT/1,1,2,4,9,20,48,115,286,719,1842,4766/	00001300
	DATA INDEX/1,1,2,5,11,28,67,171,433,1123,2924/	00001400
	DATA ZERO,UNITY,TWO,ZAPP/O.ODO,1.ODO,2.ODO,1.OD-14/	00001500
	DATA MAXORD/12/	00001600
C		00001700
C	*****	00001800
C		00001900
	DATA KPRINT/O/	00002000
C		00002100
C	*****	00002200
C		00002300
C		00002400
C		00002500
C	SUBROUTINE RKEQ IS A FORTRAN SUBROUTINE WRITTEN BY	00002600
C	M.K. HORN WHICH IMPLEMENTS THE ALGORITHM DEVELOPED	00002700
C	BY D.G. BETTIS TO GENERATE TRUNCATION ERROR COEFFI-	00002800
C	IENTS FOR RUNGE-KUTTA ALGORITHMS.	00002900
C		00003000
C	REFERENCE: BETTIS,D.G. AND M.K. HORN, 'COMPUTATION	00003100
C	OF TRUNCATION ERROR TERMS FOR RUNGE-KUTTA METHODS,'	00003200
C	TICOM REPORT 77-14, DECEMBER, 1978.	00003300
C		00003400
C	SUBROUTINE RKEQ DETERMINES THE TRUNCATION ERROR	00003500
C	COEFFICIENTS (TEC) FOR A RUNGE-KUTTA ALGORITHM HAVING	00003600
C	AN EMBEDDED PAIR OF SOLUTIONS	00003700
C		00003800
C		00003900
C		00004000
C	Y = Y + H SUM C F	00004100
C	1 0 K K	00004200
C	K=0	00004300
C		00004400
C		00004500
C		00004600
C		00004700
C	YH = Y + H SUM CH F	00004800
C	1 0 K K	00004900

C		K=0	00005000
C			00005100
C			00005200
C			00005300
C	WHERE	$F = F(T, Y)$	00005400
C		0 0 0	00005500
C			00005600
C			00005700
C		K-1	00005800
C			00005900
C		$F = F(T + A H, Y + H * \text{SUM } B_{K,L} F)$	00006000
C		K 0 K 0 L=0	00006100
C			00006200
C			00006300
C		FOR MFOLD = 0, RKEQ FORMS THE TEC FOR THE CLASSICAL RK	00006400
C		FORMULAS OF ORDER = IORDER. FOR MFOLD = M, RKEQ FORMS	00006500
C		THE TEC FOR MFOLD-RK FORMULAS OF ORDER = M + IORDER.	00006600
C			00006700
C			00006800
C			00006900
C	-----		00007000
C	OPTION .EQ. 1	COMPUTES AND PRINTS ALL TRUNCATION	00007100
C		ERROR COEFFICIENTS THROUGH ORDER =	00007200
C		IORDER	00007300
C	OPTION .EQ. 2	COMPUTES AND PRINTS ONLY T.E.C. OF	00007400
C		ORDER = IORDER	00007500
C	OPTION .EQ. 3	COMPUTES T.E.C. AS IN OPTION = 2 BUT	00007600
C		DOES NOT PRINT	00007700
C			00007800
C	-----		00007900
C			00008000
C			00008100
C		ADJUSTS INPUT PARAMETERS IF THESE ARE NOT WITHIN	00008200
C		ALLOWABLE RANGE	00008300
C			00008400
C			00008500
C		ORDER = IORDER	00008600
C		LIMITS = ITERR	00008700
C		IF (ORDER .LT. LIMITS) ORDER = LIMITS	00008800
C		IF (LS. LT. LIMIT(MAXORD)) GO TO 1	00008900
C		IF (ORDER .LE. MAXORD) GO TO 1	00009000
C		ORDER = MAXORD	00009100
C		PRINT 507,MAXORD	00009200
C	507	FORMAT(52H ORDER REQUESTED IS BEYOND CAPABILITY OF THE PROGRAM	00009300
C	1 ,/,24H	ORDER LOWERED--ORDER = ,I2)	00009400
C		IF (ITERR .LE. ORDER) GO TO 1	00009500
C		LIMITS = ORDER	00009600
C		PRINT 526,LIMITS	00009700
C	526	FORMAT(45H ITERR REQUESTED IS LARGER THAN MAXIMUM ORDER	00009800
C	1 ,/,35H	ITERR HAS BEEN REDUCED TO ORDER = ,I2)	00009900

C		00010000
	1 CONTINUE	00010100
C		00010200
	TERROR = ZERO	00010300
	OPTION = IOPT	00010400
	IF (IOPT .LE. 0 .OR. IOPT .GT. 3) OPTION = 1	00010500
	IF (LS .GE. LIMIT(ORDER)) GO TO 3	00010600
	2 CONTINUE	00010700
	ORDER = ORDER - 1	00010800
	IF (LS .LT. LIMIT(ORDER)) GO TO 2	00010900
	PRINT 505,ORDER,IORDER,LIMIT(IORDER)	00011000
	505 FORMAT(50H THE ORDER SPECIFIED HAS BEEN REDUCED TO ORDER =	00011100
	1 ,I3,/,32H BECAUSE OF INSUFFICIENT STORAGE ,/,	00011200
	2 14H FOR ORDER = ,I3,20H LS MUST BE .GE. ,I5,	00011300
	3 /,56H TERROR = SQRT(SUM(T.E.C.(I,J)*T.E.C.(I,J))) IS COMPUTED	00011400
	4 ,/,14H FOR I = ORDER)	00011500
C		00011600
	IF (LIMITS .LE. ORDER) GO TO 3	00011700
	LIMITS = ORDER	00011800
	PRINT 527,LIMITS	00011900
	527 FORMAT(45H ITERR REQUESTED IS LARGER THAN THE PROVIDED	00012000
	1,/,50H DIMENSIONING. ITERR HAS BEEN REDUCED TO ITERR = ,	00012100
	2 I2)	00012200
	3 CONTINUE	00012300
C		00012400
C		00012500
C		00012600
	IF (ORDER .GT. MAXORD) ORDER = MAXORD	00012700
C		00012800
C		00012900
C	-----	00013000
C		00013100
C	MP(J) = (MFOLD+J) D.P.	00013200
C	M(J) = J INTEGER	00013300
C	FACT(J) = J D.P.	00013400
C	MM(J) = (MFOLD+J) D.P.	00013500
C		00013600
C	INDEX--COUNTS THE NUMBER OF S(J,K) WITH A GIVEN A**K	00013700
C	AS THE FIRST TERM IN THE EXPRESSION, E.G.,	00013800
C	FOR J=7, THERE ARE 1 A**6, 1 A**4, 2 A**3,	00013900
C	4 A**2, AND 9 A**1 @S	00014000
C		00014100
C	-----	00014200
C		00014300
	X1 = A(1) - B0(1)	00014400
	JJ = 1	00014500
	550 FORMAT(15H ERROR IN BETA(,I2,10H) SUM = ,D15.7)	00014600
	IF (DABS(X1) .GE. ZAPP) PRINT 550,JJ,X1	00014700
	DO 5 J = 2,R	00014800
	X1 = A(J) - B0(J)	00014900

	JLOW = J-1	00015000
	DO 4 K = 1,JLOW	00015100
	4 X1 = X1 - B(J,K)	00015200
	IF (DABS(X1) .GE. ZAPP) PRINT 550,J,X1	00015300
	5 CONTINUE	00015400
C		00015500
	IF (KPRINT .EQ. 1) READ PRINT 499	00015600
C		00015700
C		00015800
C	SETS VALUES OF FACTORIALS USED IN THE PROGRAM.	00015900
C	ADJUSTMENTS IN THE PROGRAM TO ACCOMODATE M-FOLD	00016000
C	RUNGE-KUTTA ALGORITHMS OCCUR HERE. IF MFOLD = 0,	00016100
C	THE CLASSICAL RUNGE-KUTTA T.E.C. OCCUR	00016200
C		00016300
		00016400
	IF (MFOLD .GT. 0) GO TO 6	00016500
	EVEN = .TRUE.	00016600
	GO TO 8	00016700
	6 CONTINUE	00016800
	N1 = MFOLD / 2	00016900
	N2 = 2 * N1	00017000
	EVEN = .FALSE.	00017100
	IF (N2 .EQ. MFOLD) EVEN = .TRUE.	00017200
	8 CONTINUE	00017300
	MP(1) = DFLOAT(MFOLD)+UNITY	00017400
	M(1) = 1	00017500
	X1 = UNITY	00017600
	FACT(1) = UNITY	00017700
	DO 10 I = 2,ORDER	00017800
	X1 = X1 + UNITY	00017900
	FACT(I) = FACT(I-1)*X1	00018000
	MP(I) = MP(I-1) + UNITY	00018100
	10 M(I) = M(I-1) + 1	00018200
	M2 = 1	00018300
	M1 = 0	00018400
	11 CONTINUE	00018500
	M1 = M1 + 1	00018600
	M2 = M2*M1	00018700
	IF (M1 .LT. MFOLD+1) GO TO 11	00018800
	MM(1) = DFLOAT(M2)	00018900
	DO 12 I = 2,ORDER	00019000
	12 MM(I) = MP(I)* MM(I-1)	00019100
C		00019200
C		00019300
	IF (KPRINT .EQ. 1) PRINT 499	00019400
C		00019500
C	SETS INITIAL VALUES OF S(I,J) EQUAL TO ZERO	00019600
C	AND SETS AA(J) AND BB(J) EQUAL TO UNITY	00019700
C		00019800
	DO 14 J = 1,LS	00019900

	AA(J) = UNITY	00020000
	BB(J) = UNITY	00020100
	DO 14 K = 1,R	00020200
	14 S(J,K) = ZERO	00020300
C		00020400
	IF (OPTION .GT. 1 .AND. LIMITS .NE. 1) GO TO 21	00020500
C		00020600
C	EVALUATES T.E.C. OF ORDER 1	00020700
C		00020800
	SUM1 = UNITY/DFLOAT(MFOLD + 1) - CO	00020900
	SUM3 = UNITY/DFLOAT(MFOLD + 1) - CHO	00021000
	DO 20 I = 1,R	00021100
	SUM1 = SUM1 - C(I)	00021200
	SUM3 = SUM3 - CH(I)	00021300
	20 CONTINUE	00021400
C		00021500
	JJ1 = 1	00021600
	IF (LIMITS .EQ. 1) TERROR = SUM3*SUM3	00021700
	IF (OPTION .EQ. 3) GO TO 21	00021800
	PRINT 500,JJ1	00021900
	PRINT 501,JJ1,JJ1,SUM1,SUM3	00022000
	500 FORMAT(36H TRUNCATION ERROR TERMS X-ORDER = ,I2,2X	00022100
	1 ,//)	00022200
	501 FORMAT(2(2X,I4),2(D15.7))	00022300
C		00022400
	21 CONTINUE	00022500
C		00022600
C	SETS S(1,J) TERMS	00022700
C		00022800
	KOUNT = 1	00022900
C		00023000
	DO 26 I = 1,R	00023100
	IF (MFOLD .GT. 0) GO TO 22	00023200
	S(1,I) = A(I)	00023300
	GO TO 26	00023400
	22 CONTINUE	00023500
	IF (EVEN) GO TO 24	00023600
	S(1,I) = DABS(A(I))**MP(1)	00023700
	GO TO 26	00023800
	24 CONTINUE	00023900
	X1 = DABS(A(I))**MP(1)	00024000
	S(1,I) = DSIGN(X1,A(I))	00024100
	26 CONTINUE	00024200
C		00024300
C	EVALUATES T.E.C. FOR ORDER = KOUNT = 2,3	00024400
C		00024500
C		00024600
	AA(1) = UNITY	00024700
	BB(1) = MM(1)	00024800
	28 CONTINUE	00024900

	P = TWO + DFLOAT(MFOLD)	00025000
	PP1 = P+UNITY	00025100
30	CONTINUE	00025200
	IF (LIMITS .EQ. KOUNT) JJ1 = KOUNT - 1	00025300
	IF (OPTION .GT. 1 .AND. LIMITS .NE. KOUNT) GO TO 34	00025400
	JJ2 = 0	00025500
	JJ1 = KOUNT + 1	00025600
	PRINT 500, JJ1	00025700
	DO 33 K = 1, KOUNT	00025800
	JJ2 = JJ2 + 1	00025900
	SUM1 = UNITY/(AA(K)*P)	00026000
	SUM3 = SUM1	00026100
	DO 32 I = 1, R	00026200
	SUM1 = SUM1 - C(I)*S(K, I)	00026300
	SUM3 = SUM3 - CH(I)*S(K, I)	00026400
32	CONTINUE	00026500
	IF (LIMITS .EQ. KOUNT) TERROR = TERROR + SUM3*SUM3	00026600
	IF (OPTION .EQ. 3) GO TO 33	00026700
	PRINT 501, JJ1, JJ2, SUM1, SUM3	00026800
33	CONTINUE	00026900
C		00027000
34	CONTINUE	00027100
C		00027200
	IF (KOUNT .EQ. 2) GO TO 38	00027300
C		00027400
C	SETS S(1, J), S(2, J) FOR THIRD ORDER T.E.C.	00027500
C		00027600
	KOUNT = 2	00027700
	P = P + UNITY	00027800
	PP1 = PP1 + UNITY	00027900
	DO 35 I = 2, R	00028000
	S(2, I) = ZERO	00028100
	IM1 = I-1	00028200
	DO 35 J = 1, IM1	00028300
35	S(2, I) = S(2, I) + B(I, J)*S(1, J)	00028400
	DO 36 I = 1, R	00028500
36	S(1, I) = S(1, I)*A(I)	00028600
	AA(2) = TWO	00028700
	BB(1) = MM(2)	00028800
	BB(2) = MM(1)	00028900
	GO TO 30	00029000
38	CONTINUE	00029100
	IF (ORDER .LE. 3) GO TO 182	00029200
	LIM1 = 3	00029300
C		00029400
C	EVALUATES T.E.C. FOR ORDERS GREATER THAN THREE	00029500
C		00029600
	DO 180 J = 4, ORDER	00029700
	P = P + UNITY	00029800
	PP1 = P + UNITY	00029900

	PM1 = P - UNITY	00030000
	PM2 = P - TWO	00030100
	IF (KPRINT .EQ. 1) READ 497,II	00030200
	LIM1 = LIM1 + 1	00030300
	LIMA = LIMIT(J-1)	00030400
	LIMB = LIMA	00030500
C		00030600
C	COMPUTES S(1,I)--ALL OTHER S(J,K) TERMS INVOLVING A	00030700
C	LEADING ALPHA ARE ALREADY DETERMINED	00030800
C	EXCEPT FOR THE POWER OF ALPHA WHICH	00030900
C	IS DETERMINED BY IN INDEX AND J	00031000
C		00031100
C	AA(1) = AA(1)	00031200
	BB(1) = BB(1) * MP(LIM1-1)	00031300
	DO 42 I = 1,R	00031400
	42 S(1,I) = S(1,I)*A(I)	00031500
C		00031600
C	LIM1 = INTEGER P	00031700
C		00031800
C		00031900
C	BETA TERMS	00032000
C		00032200
	MARKB = LIMA+1	00032300
	DO 61 I = 2,R	00032400
	S(MARKB,I) = ZERO	00032500
	IM1 = I-1	00032600
	DO 61 K = 1,IM1	00032700
	61 S(MARKB,I) = S(MARKB,I)+B(I,K)*A(K)**(MFOLD+LIM1-2)	00032800
	AA(MARKB)=PM1	00032900
	BB(MARKB) = MM(LIM1-2)	00033000
	IND2 = 1	00033100
	IND1 = MARKB	00033200
	LL = LIM1 - 4	00033300
	IF (LIM1 .EQ. 4) GO TO 66	00033400
	DO 65 K = 1,LL	00033500
	LL1 = INDEX(K+1)	00033600
	IPOW = LL-K+1	00033700
	DO 65 KK = 1,LL1	00033800
	IND1 = IND1 + 1	00033900
	IND2 = IND2 + 1	00034000
	DO 64 I = 2,R	00034100
	S(IND1,I) = ZERO	00034200
	IM1 = I-1	00034300
	DO 64 L = 1,IM1	00034400
	64 S(IND1,I) = S(IND1,I)+B(I,L)*S(IND2,L)*A(L)**M(IPOW)	00034500
	BB(IND1) = BB(IND2)*FACT(IPOW)	00034600
	65 AA(IND1) = AA(IND2)*PM1	00034700
	66 CONTINUE	00034800
	LL = LIMB - IND2	00034900

	DO 68 K = 1,LL	00035000
	IND1 = IND1 + 1	00035100
	IND2 = IND2 + 1	00035200
	DO 67 I = 2, N	00035300
	S(IND1,I) = ZERO	00035400
	IM1 = I-1	00035500
	DO 67 L = 1,IM1	00035600
	67 S(IND1,I) = S(IND1,I)+B(I,L)*S(IND2,L)	00035700
	BB(IND1) = BB(IND2)	00035800
	68 AA(IND1) = AA(IND2)*PM1	00035900
	883 CONTINUE	00036000
	JM3 = J - 3	00036100
	GO TO (150,100,105,110,115,120,125,130,135),JM3	00036200
		00036300
C		00036400
C	CROSS PRODUCT TERMS	00036500
C		00036600
	100 CONTINUE	00036700
C		00036800
C	5 TH ORDER TERMS	00036900
C		00037000
	IND = 2*LIMIT(4)+1	00037100
	CALL CROSS(LS,R,S,AA,BB,IND,2,2,0,0)	00037200
	GO TO 150	00037300
C		00037400
C	6 TH ORDER TERMS	00037500
	105 CONTINUE	00037600
	IND = 2*LIMIT(5)+1	00037700
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,3,4)	00037800
	GO TO 150	00037900
		00038000
		00038100
C		00038200
C	7 TH ORDER TERMS	00038300
C		00038400
	110 CONTINUE	00038500
	IND = 2*LIMIT(6)+1	00038600
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,5,8)	00038700
	CALL CROSS(LS,R,S,AA,BB,IND,2,3,0,0)	00038800
	CALL CROSS(LS,R,S,AA,BB,IND,3,2,0,0)	00038900
	CALL CROSS(LS,R,S,AA,BB,IND,4,2,0,0)	00039000
	CALL CROSS(LS,R,S,AA,BB,IND,3,1,4,4)	00039100
	GO TO 150	00039200
C		00039300
C	8 TH ORDER TERMS	00039400
C		00039500
	115 CONTINUE	00039600
	IND = 2*LIMIT(7)+1	00039700
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,10,18)	00039800
	CALL CROSS(LS,R,S,AA,BB,IND,3,1,5,8)	00039900
	CALL CROSS(LS,R,S,AA,BB,IND,4,1,5,8)	00039900

	CALL CROSS(LS,R,S,AA,BB,IND,2,2,3,4)	00040000
	GO TO 150	00040100
C		00040200
C	9 TH ORDER TERMS	00040300
	120 CONTINUE	00040400
	IND = 2*LIMIT(8)+1	00040500
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,21,40)	00040600
	CALL CROSS(LS,R,S,AA,BB,IND,3,1,10,13)	00040700
	CALL CROSS(LS,R,S,AA,BB,IND,4,1,10,18)	00040800
	DO 121 K = 5,8	00040900
	121 CALL CROSS(LS,R,S,AA,BB,IND,K,1,K,8)	00041000
	CALL CROSS(LS,R,S,AA,BB,IND,9,1,5,8)	00041100
	CALL CROSS(LS,R,S,AA,BB,IND,2,4,0,0)	00041200
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,46,48)	00041300
	GO TO 150	00041400
C		00041500
C	10 TH ORDER TERMS	00041600
C		00041700
	125 CONTINUE	00041800
	IND = 2*LIMIT(9) + 1	00041900
C		00042000
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,49,96)	00042100
	CALL CROSS(LS,R,S,AA,BB,IND,3,1,21,40)	00042200
	CALL CROSS(LS,R,S,AA,BB,IND,4,1,21,40)	00042300
	DO 126 K = 5,9	00042400
	126 CALL CROSS(LS,R,S,AA,BB,IND,K,1,10,18)	00042500
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,106,113)	00042600
	CALL CROSS(LS,R,S,AA,BB,IND,2,3,3,4)	00042700
	CALL CROSS(LS,R,S,AA,BB,IND,3,3,0,0)	00042800
	CALL CROSS(LS,R,S,AA,BB,IND,4,3,0,0)	00042900
	CALL CROSS(LS,R,S,AA,BB,IND,4,2,3,3)	00043000
	CALL CROSS(LS,R,S,AA,BB,IND,3,2,4,4)	00043100
C		00043200
	GO TO 150	00043300
C		00043400
	130 CONTINUE	00043500
C		00043600
C	11TH ORDER TERMS	00043700
C		00043800
	IND = 2*LIMIT(10) + 1	00043900
C		00044000
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,116,230)	00044100
	CALL CROSS(LS,R,S,AA,BB,IND,3,1,49,96)	00044200
	CALL CROSS(LS,R,S,AA,BB,IND,4,1,49,96)	00044300
	DO 131 K = 5,8	00044400
	131 CALL CROSS(LS,R,S,AA,BB,IND,K,1,21,40)	00044500
	DO 132 K = 10,18	00044600
	132 CALL CROSS(LS,R,S,AA,BB,IND,K,1,K,18)	00044700
	CALL CROSS(LS,R,S,AA,BB,IND,2,2,21,40)	00044800
	CALL CROSS(LS,R,S,AA,BB,IND,19,1,10,18)	00044900

	CALL CROSS(LS,R,S,AA,BB,IND,20,1,10,18)	00045000
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,269,278)	00045100
	DO 133 K = 46,48	00045200
133	CALL CROSS(LS,R,S,AA,BB,IND,K,1,5,8)	00045300
	CALL CROSS(LS,R,S,AA,BB,IND,2,3,5,8)	00045400
	CALL CROSS(LS,R,S,AA,BB,IND,2,2,46,48)	00045500
	CALL CROSS(LS,R,S,AA,BB,IND,2,5,0,0)	00045600
C	GO TO 150	00045700
C		00045800
C	12TH ORDER TERMS	00045900
C		00046000
C	135 CONTINUE	00046100
C		00046200
C	IND = 2*LIMIT(11) + 1	00046300
C		00046400
C		00046500
	CALL CROSS(LS,R,S,AA,BB,IND,2,1,287,572)	00046600
	CALL CROSS(LS,R,S,AA,BB,IND,3,1,116,230)	00046700
	CALL CROSS(LS,R,S,AA,BB,IND,4,1,116,230)	00046800
	DO 141 K = 5,8	00046900
141	CALL CROSS(LS,R,S,AA,BB,IND,K,1,49,96)	00047000
	DO 142 K = 10,18	00047100
142	CALL CROSS(LS,R,S,AA,BB,IND,K,1,21,40)	00047200
	CALL CROSS(LS,R,S,AA,BB,IND,2,2,49,96)	00047300
	CALL CROSS(LS,R,S,AA,BB,IND,19,1,21,40)	00047400
	CALL CROSS(LS,R,S,AA,BB,IND,20,1,21,40)	00047500
	DO 143 K = 41,48	00047600
143	CALL CROSS(LS,R,S,AA,BB,IND,K,1,10,18)	00047700
	CALL CROSS(LS,R,S,AA,BB,IND,114,1,5,8)	00047800
	CALL CROSS(LS,R,S,AA,BB,IND,115,1,5,8)	00047900
	DO 144 K = 269,278	00048000
144	CALL CROSS(LS,R,S,AA,BB,IND,K,1,3,4)	00048100
	CALL CROSS(LS,R,S,AA,BB,IND,3,3,2,2)	00048200
	CALL CROSS(LS,R,S,AA,BB,IND,4,3,2,2)	00048300
	CALL CROSS(LS,R,S,AA,BB,IND,3,2,20,20)	00048400
	CALL CROSS(LS,R,S,AA,BB,IND,4,2,19,19)	00048500
	CALL CROSS(LS,R,S,AA,BB,IND,2,4,3,4)	00048600
150	CONTINUE	00048700
		00048800
C		00048900
C	TEMPORARY INSERT TO CHECK VALUES OF AA AND BB COEFF	00049000
C		00049100
C	LL = LIMIT(LIM1)	00049200
C	IFAKE = 0	00049300
C	DO 153 K = 1,LL	00049400
C	IFAKE = IFAKE + 1	00049500
C	IF (IFAKE .LT. 40) GO TO 153	00049600
C	IF (KPRINT .EQ. 1) READ 497,II	00049700
C	IFAKE = 0	00049800
C	153 PRINT 506,K,AA(K),K,BB(K)	00049900

C	506	FORMAT(4H AA(,I4, 4H) = ,D15.7,2X,4H BB(,	00050000
C	1	I4,4H) = ,D15.7)	00050100
		IF (KPRINT .EQ. 1) PRINT 499	00050200
C			00050300
C			00050400
C			00050500
		IF (LIMITS .EQ. J) JJ1 = J - 1	00050600
		IF (OPTION .GT. 1 .AND. LIMITS .NE. J) GO TO 180	00050700
C			00050800
		JJ2 = 1	00050900
		JJ1 = J	00051000
C			00051100
C		EVALUATES FIRST T.E.C. OF ORDER J	00051200
C			00051300
		SUM1 = UNITY/(AA(1)*P)	00051400
		SUM3 = SUM1	00051500
		DO 154 I = 1,R	00051600
		SUM1 = SUM1 - C(I)*S(1,I)	00051700
		SUM3 = SUM3 - CH(I)*S(1,I)	00051800
	154	CONTINUE	00051900
		SUM1 = SUM1 / BB(1)	00052000
		SUM3 = SUM3 / BB(1)	00052100
		IF (LIMITS .EQ. J) TERROR = TERROR + SUM3*SUM3	00052200
		IF (OPTION .EQ. 3) GO TO 155	00052300
		PRINT 501, JJ1, JJ2, SUM1, SUM3	00052400
	155	CONTINUE	00052500
C			00052600
C			00052700
C		EVALUATES T.E.C. FOR S(I,J) TERMS WITH ALPHA AS	00052800
C		LEADING COEFFICIENT (I .NE. 2)	00052900
C			00053000
		IFAKE = 1	00053100
		K = 1	00053200
		KNT = 2	00053300
		IPOW = LIM1 - 3	00053400
		LIMD = INDEX(KNT)	00053500
	156	CONTINUE	00053600
		DO 159 KK = 1, LIMD	00053700
		K = K + 1	00053800
		SUM1 = UNITY/(AA(K)*P)	00053900
		SUM3 = SUM1	00054000
		DO 157 I = 1,R	00054100
		SUM1 = SUM1 - C(I)*A(I)**IPOW*S(K,I)	00054200
		SUM3 = SUM3 - CH(I)*A(I)**IPOW*S(K,I)	00054300
	157	CONTINUE	00054400
		SUM1 = SUM1 / (BB(K)*FACT(IPOW))	00054500
		SUM3 = SUM3 / (BB(K)*FACT(IPOW))	00054600
		IF (LIMITS .EQ. J) TERROR = TERROR + SUM3*SUM3	00054700
		IF (OPTION .EQ. 3) GO TO 159	00054800
		JJ2 = JJ2 + 1	00054900

	IFAKE = IFAKE + 1	00055000
	IF (IFAKE .LT. 40) GO TO 158	00055100
	IFAKE = 0	00055200
	IF (KPRINT .EQ. 1) PRINT 499	00055300
158	CONTINUE	00055400
497	FORMAT(I3)	00055500
	PRINT 501, JJ1, JJ2, SUM1, SUM3	00055600
159	CONTINUE	00055700
C		00055800
	KNT = KNT + 1	00055900
	LIMD = INDEX(KNT)	00056000
	IPOW = IPOW - 1	00056100
	IF (IPOW .GE. 1) GO TO 156	00056200
C		00056300
	LIMD = LIMIT(LIM1) - LIMA	00056400
C		00056500
C	EVALUATES T.E.C. FOR S(I,J) TERMS WITH BETA AS	00056600
C	LEADING COEFFICIENT	00056700
C		00056800
	DO 162 KK = 1, LIMD	00056900
	K = K + 1	00057000
	SUM1 = UNITY/(AA(K)*P)	00057100
	SUM3 = SUM1	00057200
	DO 160 I = 1, R	00057300
	SUM1 = SUM1 - C(I)*S(K,I)	00057400
	SUM3 = SUM3 - CH(I)*S(K,I)	00057500
160	CONTINUE	00057600
	SUM1 = SUM1 / BB(K)	00057700
	SUM3 = SUM3 / BB(K)	00057800
	IF (LIMITS .EQ. J) TERROR = TERROR + SUM3*SUM3	00057900
	IF (OPTION .EQ. 3) GO TO 162	00058000
	IFAKE = IFAKE + 1	00058100
	IF (IFAKE .LT. 40) GO TO 161	00058200
	IFAKE = 0	00058300
	IF (KPRINT .EQ. 1) PRINT 499	00058400
161	CONTINUE	00058500
	JJ2 = JJ2 + 1	00058600
C	PRINT 556, K, LIM1, AA(K), P, PP1	00058700
556	FORMAT(2(2X, I4), 3(2X, D15.7))	00058800
	PRINT 501, JJ1, JJ2, SUM1, SUM3	00058900
162	CONTINUE	00059000
	IF (KPRINT .EQ. 1) PRINT 499	00059100
499	FORMAT(//)	00059200
180	CONTINUE	00059300
182	CONTINUE	00059400
	TERROR = DSQRT(TERROR)	00059500
	RETURN	00059600
	END	00059700

```

SUBROUTINE CROSS(LS,R,S,AA,BB,INDEX,TERM1,POWER,TERM2,
1  TERM3)
  INTEGER TERM1,TERM2,TERM3,POWER,R
  DOUBLE PRECISION S(LS,R),AA(LS),BB(LS),FACT(7)
C
  DATA FACT/1.0D0,2.0D0,6.0D0,24.0D0,
1  120.0D0,720.0D0,5040.0D0/
C
C
C
  IF (TERM2 .EQ. 0) GO TO 20
C
C  COMPUTES S(INDEX+J,I)=S(TERM1,I)**POWER * S(TERM2+J,I)
C  FOR J=0,1,...,TERM3-TERM2
C
  KK = -1
  DO 10 K = TERM2,TERM3
  KK = KK + 1
  INDX = INDEX + KK
  AA(INDX) = AA(TERM1)**POWER * AA(K)
  IPOW = POWER
  IF (TERM1 .EQ. K) IPOW = IPOW + 1
  BB(INDX) = BB(TERM1)**POWER * BB(K) *FACT(IPOW)
  DO 10 I = 2,R
10  S(INDX,I) = S(TERM1,I)**POWER * S(K,I)
  INDEX = INDEX + TERM3 - TERM2 + 1
C
C
  RETURN
C
C  COMPUTES S(INDEX,I) = S(TERM1,I)**POWER
C
20  CONTINUE
  AA(INDEX) = AA(TERM1)**POWER
  BB(INDEX) = BB(TERM1)**POWER * FACT(POWER)
  DO 25 I = 2,R
25  S(INDEX,I) = S(TERM1,I)**POWER
  INDEX = INDEX + 1
C
C
  RETURN
  END

```