

## Chapter 2

# Real Symmetric Matrices

### 2.1 Introduction

The FORTRAN codes in this chapter address the question of computing distinct eigenvalues and corresponding eigenvectors of real symmetric matrices, using a single-vector Lanczos procedure. For a given real symmetric matrix  $A$ , these codes compute real scalars  $\lambda$  and corresponding real vectors  $x \neq 0$ , such that

$$Ax = \lambda x. \tag{2.1.1}$$

**Definition 1** *The real  $n \times n$  matrix  $A \equiv (a_{ij})$ ,  $1 \leq i, j \leq n$ , is a real symmetric matrix if and only if for every  $i, j$ ,  $a_{ij} = a_{ji}$ .*

Real symmetric matrices are discussed in detail in Stewart [24]. Properties which we use are:

1. Real symmetric matrices have complete eigensystems. That is, the dimension of the eigenspace corresponding to any given eigenvalue of the given matrix  $A$  is the same as the multiplicity of that eigenvalue as a root of the characteristic polynomial of  $A$ .
2. For any two distinct eigenvalues of  $A$ ,  $\lambda$  and  $\mu$ , and corresponding eigenvectors  $x$  and  $y$ ,  $x^T y = 0$ . Thus, eigenvectors corresponding to different eigenvalues are orthogonal, and we can construct an eigenvector basis which is orthonormal. Vectors are orthonormal if they are orthogonal and each has a Euclidean norm of 1. (The Euclidean norm of a vector is just the square root of the sum of the squares of its components.)
3. Small perturbations in the matrix cause only small perturbations in the eigenvalues. Of the classes of matrices which we consider, the class of real symmetric matrices is the most well-behaved and thus the 'easiest'.

The Lanczos codes contained in this chapter correspond to the most straight-forward implementation of the Lanczos recursion included in this book. These codes can be used to compute either a very few or very many of the distinct eigenvalues of the given real symmetric matrix. As the documentation in the next section indicates, the  $A$ -multiplicity of a given computed 'good' Lanczos eigenvalue can be obtained only with additional computation, and the modifications required to do this additional computation are not included in these versions of the codes. This implementation uses the basic Lanczos recursion given in Eqns (1.2.1) and (1.2.2) in Section 1.2 of Chapter 1 to generate a family of real symmetric, tridiagonal

matrices ( $T$ -matrices) whose sizes are specified by the user. There is no reorthogonalization of the Lanczos vectors at any stage in any of the computations.

LEVAL, the main program for the real symmetric eigenvalue computations, calls the subroutine BISEC to compute eigenvalues of the user-specified Lanczos tridiagonal matrices on the user-specified intervals. BISEC simultaneously computes these  $T$ -eigenvalues with their  $T$ -multiplicities and sorts the computed  $T$ -eigenvalues into two classes, the 'good'  $T$ -eigenvalues and the 'spurious'  $T$ -eigenvalues. The 'good'  $T$ -eigenvalues are accepted as approximations to eigenvalues of the user-specified matrix  $A$ . The accuracy of these 'good'  $T$ -eigenvalues as eigenvalues of  $A$  is then estimated using error estimates computed by subroutine INVERR. Error estimates are computed only for isolated 'good'  $T$ -eigenvalues. All other 'good'  $T$ -eigenvalues are assumed to have converged. If convergence has not yet occurred and a larger Lanczos matrix has been specified by the user, the program will continue on to a larger Lanczos matrix, repeating the above procedure on this larger matrix.

Once the eigenvalues have been computed accurately enough, the user can select a subset of the 'converged' eigenvalues for which eigenvectors are to be computed. The main program LEVEC, for computing eigenvectors of real symmetric matrices, is then used to compute these desired eigenvectors.

All computations are in double precision real arithmetic. The user must supply a subroutine USPEC which defines and initializes the user-specified matrix  $A$  and a subroutine CMATV which computes matrix-vector multiplies  $Ax$  for any given vector  $x$ . These subroutines must be constructed in such a way as to take advantage of the sparsity (and/or structure) of the user-supplied  $A$ -matrix and such that these computations are done accurately. More details about these real symmetric single-vector Lanczos procedures are given in Chapter 4 of Volume 1 of this book.



C		LEV00520
C	HERMITIAN MATRICES:	LEV00530
C		LEV00540
C	GIVEN A HERMITIAN MATRIX A OF ORDER N THE THREE SETS OF	LEV00550
C	FORTRAN FILES LABELLED HLEVAL, LESUB, AND HLEMULT CAN BE USED	LEV00560
C	TO COMPUTE DISTINCT EIGENVALUES IN USER-SPECIFIED INTERVALS.	LEV00570
C		LEV00580
C	CORRESPONDING EIGENVECTORS FOR SELECTED, COMPUTED EIGENVALUES	LEV00590
C	CAN BE COMPUTED USING THE SETS OF PROGRAMS LABELLED HLEVEC,	LEV00600
C	LESUB, AND HLEMULT.	LEV00610
C		LEV00620
C		LEV00630
C	FACTORED INVERSES OF REAL SYMMETRIC MATRICES:	LEV00640
C		LEV00650
C	GIVEN A REAL SYMMETRIC MATRIX A, THE LANCZOS RECURSION IS	LEV00660
C	APPLIED TO THE INVERSE OF A, USING A FACTORIZATION	LEV00670
C	OF A. THE SETS OF FILES LIVAL, LESUB, AND LIMULT	LEV00680
C	CAN BE USED TO COMPUTE THE DISTINCT EIGENVALUES OF THE	LEV00690
C	INVERSE OF THE A-MATRIX AND OF A IN USER-SPECIFIED	LEV00700
C	INTERVALS. THE PROGRAMS ACTUALLY ALLOW ONE TO WORK WITH	LEV00710
C	ANY MATRIX $B = PCP'$ WHERE $C = SO*A + SHIFT*I$ , WHERE	LEV00720
C	SO AND SHIFT ARE SCALARS CHOSEN BY THE USER AND P IS A	LEV00730
C	PERMUTATION MATRIX CHOSEN SUCH THAT THE FACTORIZATION	LEV00740
C	OF THE B-MATRIX RETAINS SPARSITY. IN THE	LEV00750
C	SAMPLE LIMULT SUBROUTINES PROVIDED, SO AND SHIFT MUST BE	LEV00760
C	CHOSEN SO THAT THE RESULTING B-MATRIX IS POSITIVE DEFINITE,	LEV00770
C	AND THE CHOLESKY FACTORS ARE USED TO SOLVE $B*U = V$ .	LEV00780
C	HOWEVER, THE USER CAN EASILY REPLACE THE SAMPLE USPEC AND	LEV00790
C	BSOLV SUBROUTINES PROVIDED BY SUBROUTINES THAT ALLOW THE	LEV00800
C	GENERAL FACTORIZATION $L*D*(L-TRANSPOSE)$ . THESE LANCZOS	LEV00810
C	PROGRAMS APPLY THE LANCZOS RECURSION TO B-INVERSE, USING	LEV00820
C	THE FACTORIZATION PROVIDED. OPTIONAL PREPROCESSING PROGRAMS	LEV00830
C	PERMUT, LORDER, LFACT, AND LTEST ARE PROVIDED FOR SET-UP PURPOSES.	LEV00840
C	PERMUT USES THE SPARSPAK PACKAGE OF A. GEORGE, J. LIU AND	LEV00850
C	E. NG TO OBTAIN A REORDERING OF THE GIVEN MATRIX THAT	LEV00860
C	PRESERVES SPARSENESS ON SUBSEQUENT FACTORIZATION. LORDER	LEV00870
C	CAN BE USED TO REORDER A GIVEN MATRIX, USING A GIVEN	LEV00880
C	PERMUTATION. LFACT CAN BE USED TO COMPUTE THE CHOLESKY	LEV00890
C	FACTORS OF A GIVEN POSITIVE DEFINITE B-MATRIX. LTEST CAN	LEV00900
C	BE USED TO ESTIMATE THE NUMERICAL CONDITION OF THE	LEV00910
C	B-MATRIX.	LEV00920
C		LEV00930
C	CORRESPONDING EIGENVECTORS FOR SELECTED, COMPUTED	LEV00940
C	EIGENVALUES CAN BE COMPUTED USING THE SETS OF FILES	LEV00950
C	LABELLED LIVEC, LESUB, AND LIMULT.	LEV00960
C		LEV00970
C	GENERALIZED REAL SYMMETRIC PROBLEMS:	LEV00980
C		LEV00990
C	GIVEN 2 REAL SYMMETRIC MATRICES A AND B WHERE IN ADDITION B IS	LEV01000
C	POSITIVE DEFINITE AND ITS CHOLESKY FACTORS ARE AVAILABLE,	LEV01010
C	THE SETS OF FILES LGVAL, LGMULT, AND LESUB CAN BE USED	LEV01020
C	TO COMPUTE THE DISTINCT EIGENVALUES OF THE GENERALIZED	LEV01030
C	PROBLEM $A*X = EVAL*B*X$ .	LEV01040
C		LEV01050
C	CORRESPONDING EIGENVECTORS CAN BE COMPUTED USING THE PROGRAMS	LEV01060

C LGVEC, LGMULT, AND LESUB. NOTE THAT THE PREPROCESSING PROGRAMS LEV01070  
 C AVAILABLE FOR USE IN CASE (3) (PERMUT, LORDER, LFACT, AND LTEST) LEV01080  
 C CAN ALSO BE USED IN THIS CASE TO OBTAIN A SUITABLE PERMUTATION, LEV01090  
 C AND A FACTORIZATION OF THE RESULTING B-MATRIX. THE A-MATRIX LEV01100  
 C CAN THEN BE PERMUTED USING LORDER. LEV01110  
 C LEV01120  
 C LEV01130  
 C THESE PROGRAMS ALL USE LANCZOS TRIDIAGONALIZATION WITHOUT LEV01140  
 C REORTHOGONALIZATION TO GENERATE REAL SYMMETRIC TRIDIAGONAL LEV01150  
 C MATRICES, T(1,MEV), OF ORDER MEV. SUBSETS OF THE EIGENVALUES OF LEV01160  
 C THESE T-MATRICES, LABELLED AS THE 'GOOD EIGENVALUES', YIELD LEV01170  
 C APPROXIMATIONS TO THE DESIRED EIGENVALUES. CORRESPONDING LEV01180  
 C RITZ VECTORS ARE APPROXIMATIONS TO THE DESIRED EIGENVECTORS. LEV01190  
 C NOTE THAT FOR CASE (4) THE GENERALIZED LANCZOS RECURSION LEV01200  
 C  $B * V(I+1) * BETA(I+1) = A * V(I) - B * V(I) * ALPHA(I) - B * V(I-1) * BETA(I)$  LEV01210  
 C IS USED, ALONG WITH THE B-NORM. LEV01220  
 C LEV01230  
 C THE IDEAS USED IN THESE PROGRAMS ARE DISCUSSED IN THE FOLLOWING LEV01240  
 C REFERENCES. LEV01250  
 C LEV01260  
 C 1. JANE CULLUM AND RALPH A. WILLOUGHBY, LANCZOS ALGORITHMS LEV01270  
 C FOR LARGE SYMMETRIC MATRICES, VOLUME ?, PROGRESS IN LEV01280  
 C SCIENTIFIC COMPUTING, EDITORS, G. GOLUB, H.O. KREISS, LEV01290  
 C S. ARBARBANEL, AND R. GLOWINSKI, BIRKHAUSER BOSTON INC., LEV01300  
 C CAMBRIDGE, MASSACHUSETTS, 1983. LEV01310  
 C LEV01320  
 C 2. JANE CULLUM AND RALPH A. WILLOUGHBY, COMPUTING EIGENVECTORS LEV01330  
 C (AND EIGENVALUES) OF LARGE, SYMMETRIC MATRICES USING LEV01340  
 C LANCZOS TRIDIAGONALIZATION, LECTURE NOTES IN MATHEMATICS, LEV01350  
 C 773, NUMERICAL ANALYSIS PROCEEDINGS, DUNDEE 1979, EDITED BY LEV01360  
 C G. A. WATSON, SPRINGER-VERLAG, (1980), BERLIN, PP.46-63. LEV01370  
 C LEV01380  
 C 3. IBID, LANCZOS AND THE COMPUTATION IN SPECIFIED INTERVALS OF LEV01390  
 C THE SPECTRUM OF LARGE SPARSE, REAL SYMMETRIC MATRICES, SPARSE LEV01400  
 C MATRIX PROCEEDINGS 1978, ED. I.S. DUFF AND G. W. STEWART, LEV01410  
 C SIAM, PHILADELPHIA, PP.220-255, 1979. LEV01420  
 C LEV01430  
 C 4. IBID, COMPUTING EIGENVALUES OF VERY LARGE SYMMETRIC MATRICES- LEV01440  
 C AN IMPLEMENTATION OF A LANCZOS ALGORITHM WITHOUT LEV01450  
 C REORTHOGONALIZATION, J. COMPUT. PHYS. 44(1981), 329-358. LEV01460  
 C LEV01470  
 C LEV01480  
 C-----PORTABILITY-----LEV01490  
 C LEV01500  
 C LEV01510  
 C PROGRAMS WERE TESTED FOR PORTABILITY USING THE PFORT VERIFIER. LEV01520  
 C FOR DETAILS OF THE VERIFIER SEE FOR EXAMPLE, B. G. RYDER AND LEV01530  
 C A. D. HALL, "THE PFORT VERIFIER", COMPUTING SCIENCE TECHNICAL LEV01540  
 C REPORT 12, BELL LABORATORIES, MURRAY HILL, NEW JERSEY 07974, LEV01550  
 C (REVISED), JANUARY 1981. LEV01560  
 C LEV01570  
 C WITH THE EXCEPTION OF THE PROGRAMS FOR HERMITIAN MATRICES WHICH LEV01580  
 C ARE NOT PORTABLE BECAUSE OF THEIR USE OF COMPLEX\*16 VARIABLES, LEV01590  
 C THE OTHER PROGRAMS INCLUDED ARE PORTABLE EXCEPT FOR A FEW LEV01600  
 C CONSTRUCTIONS WHICH, IF NECESSARY, WILL HAVE TO BE MODIFIED LEV01610

C	BY THE USER FOR THE PARTICULAR COMPUTER BEING USED.	LEV01620
C		LEV01630
C	NONPORTABLE CONSTRUCTIONS:	LEV01640
C		LEV01650
C	REAL SYMMETRIC MATRICES:	LEV01660
C	IN LEVAL AND IN LEVEC	LEV01670
C	1. DATA/MACHEP STATEMENT	LEV01680
C	2. ALL READ(5,*) STATEMENTS (FREE FORMAT)	LEV01690
C	3. FORMAT(20A4) USED FOR THE EXPLANATORY HEADER ARRAY, EXPLAN	LEV01700
C	4. FORMAT(4Z20) USED TO READ AND WRITE ALPHA/BETA FILES.	LEV01710
C	IN LEMULT	LEV01720
C	1. IN CMATV AND USPEC THE ENTRY THAT PASSES THE STORAGE	LEV01730
C	LOCATIONS OF THE ARRAYS DEFINING THE USER-SPECIFIED	LEV01740
C	MATRIX.	LEV01750
C	2. IN THE SAMPLE USPEC PROVIDED: FREE FORMAT (8,*),	LEV01760
C	THE FORMAT (20A4), AND DATA/MACHEP STATEMENT.	LEV01770
C		LEV01780
C	HERMITIAN MATRICES:	LEV01790
C	IN HLEVAL AND IN HLEVEC	LEV01800
C	1. DATA/MACHEP STATEMENT	LEV01810
C	2. ALL READ(5,*) STATEMENTS (FREE FORMAT)	LEV01820
C	3. FORMAT(20A4) USED FOR THE EXPLANATORY HEADER ARRAY, EXPLAN	LEV01830
C	4. COMPLEX*16 VARIABLES AND FUNCTIONS SUCH AS DCMPLEX.	LEV01840
C	5. FORMAT (4Z20) USED TO READ AND WRITE ALPHA/BETA FILES.	LEV01850
C	IN HLEMULT	LEV01860
C	1. IN CMATV AND USPEC THE ENTRY THAT PASSES THE STORAGE	LEV01870
C	LOCATIONS OF THE ARRAYS DEFINING THE USER-SPECIFIED	LEV01880
C	MATRIX.	LEV01890
C	2. COMPLEX*16 VARIABLES AND FUNCTIONS SUCH AS DCMPLEX.	LEV01900
C	3. IN THE SAMPLE USPEC PROVIDED: FREE FORMAT (8,*),	LEV01910
C	THE FORMAT (20A4), AND DATA/MACHEP STATEMENT.	LEV01920
C		LEV01930
C	FACTORED INVERSES OF REAL SYMMETRIC MATRICES:	LEV01940
C	IN LIVAL AND IN LIVEC	LEV01950
C	1. DATA/MACHEP STATEMENT	LEV01960
C	2. ALL READ(5,*) STATEMENTS (FREE FORMAT)	LEV01970
C	3. FORMAT(20A4) USED FOR THE EXPLANATORY HEADER ARRAY, EXPLAN	LEV01980
C	4. FORMAT(4Z20) USED TO READ AND WRITE ALPHA/BETA FILES.	LEV01990
C	IN LIMULT	LEV02000
C	1. IN USPEC AND BSOLV, THE ENTRIES THAT PASS	LEV02010
C	THE STORAGE LOCATIONS OF THE ARRAYS DEFINING THE	LEV02020
C	USER-SPECIFIED MATRIX.	LEV02030
C	2. IN THE SAMPLE USPEC SUBROUTINES PROVIDED:	LEV02040
C	FORMATS (20A4) AND (4Z20), FREE FORMAT (8,*), AND	LEV02050
C	DATA/MACHEP STATEMENTS.	LEV02060
C		LEV02070
C		LEV02080
C	GENERALIZED SYMMETRIC PROBLEM, B-MATRIX POSITIVE	LEV02090
C	DEFINITE AND CHOLESKY FACTORS AVAILABLE:	LEV02100
C	IN LGVAL AND IN LGVEC	LEV02110
C	1. DATA/MACHEP STATEMENT	LEV02120
C	2. ALL READ(5,*) STATEMENTS (FREE FORMAT)	LEV02130
C	3. FORMAT(20A4) USED FOR THE EXPLANATORY HEADER ARRAY, EXPLAN	LEV02140
C	4. FORMAT(4Z20) USED TO READ AND WRITE ALPHA/BETA FILES.	LEV02150
C	IN LGMULT	LEV02160

C	1. IN USPECA, USPECB, AMATV AND LSOLV THE ENTRIES	LEV02170
C	THAT PASS THE STORAGE LOCATIONS OF THE ARRAYS DEFINING	LEV02180
C	THE USER-SPECIFIED MATRICES.	LEV02190
C	2. IN THE SAMPLE USPECA AND USPECB SUBROUTINES PROVIDED:	LEV02200
C	FORMATS (20A4) AND (4Z20), FREE FORMAT (8,*), AND	LEV02210
C	DATA/MACHEP STATEMENTS.	LEV02220
C		LEV02230
C	ALL 4 CASES USE THE FORTRAN FILE LESUB:	LEV02240
C	IN LESUB ALL STATEMENTS ARE PORTABLE EXCEPT FOR:	LEV02250
C	(1) THE ENTRY IN SUBROUTINE LPERM THAT PASSES THE	LEV02260
C	PERMUTATION FROM THE USPEC SUBROUTINE TO LPERM.	LEV02270
C	(THIS IS USED ONLY IN CASES (3) AND (4)).	LEV02280
C	(2) THE COMPLEX*16 VARIABLES AND FUNCTIONS USED IN	LEV02290
C	SUBROUTINE CINPRD. (THIS IS USED ONLY IN CASE (2)).	LEV02300
C		LEV02310
C	IN THE COMMENTS BELOW:	LEV02320
C		LEV02330
C	COMPLEX*16 = COMPLEX VARIABLE, 16 BYTES OF STORAGE	LEV02340
C	REAL*8 = REAL VARIABLE, 8 BYTES OF STORAGE	LEV02350
C	REAL*4 = REAL VARIABLE, 4 BYTES OF STORAGE	LEV02360
C	INTEGER*4 = INTEGER VARIABLE, 4 BYTES	LEV02370
C		LEV02380
C		LEV02390
C	-----MATRIX SPECIFICATION-----	LEV02400
C		LEV02410
C		LEV02420
C	IN CASES (1) AND (2), SUBROUTINE USPEC IS USED TO SPECIFY THE	LEV02430
C	USER-SUPPLIED A-MATRIX. SIMILARLY, IN CASE (4) SUBROUTINES	LEV02440
C	USPECA AND USPECB DEFINE THE USER-SUPPLIED A-MATRIX AND B-MATRIX.	LEV02450
C	IN CASE (3) ((4)), SUBROUTINE USPECB DEFINES THE FACTORIZATION	LEV02460
C	OF THE MATRIX (B-MATRIX) USED BY THE LANCZOS PROCEDURE.	LEV02470
C	(IN CASE (3) THE A-MATRIX IS NOT USED DIRECTLY.)	LEV02480
C		LEV02490
C	IN CASES (1) AND (2), SUBROUTINE CMATV IS A CORRESPONDING	LEV02500
C	MATRIX-VECTOR MULTIPLY SUBROUTINE WHICH SHOULD BE DESIGNED	LEV02510
C	TO TAKE ADVANTAGE OF ANY SPECIAL PROPERTIES OF THE GIVEN	LEV02520
C	MATRIX. IN CASE (4) THIS SUBROUTINE IS NEEDED FOR THE	LEV02530
C	A-MATRIX AND THUS IS CALLED AMATV. IN CASES (3) AND (4)	LEV02540
C	SUBROUTINES THAT CAN SOLVE $B*U = V$ , USING A SPARSE	LEV02550
C	FACTORIZATION OF B ARE NEEDED. THESE SUBROUTINES ARE	LEV02560
C	CALLED RESPECTIVELY, BSOLV AND LSOLV. IN ALL CASES,	LEV02570
C	ANY MATRIX-VECTOR MULTIPLY AND SOLVE SUBROUTINES USED	LEV02580
C	MUST BE DESIGNED TO COMPUTE RAPIDLY AND ACCURATELY.	LEV02590
C		LEV02600
C	IN ALL CASES:	LEV02610
C	SUBROUTINE USPEC(A OR B) HAS THE CALLING SEQUENCE	LEV02620
C		LEV02630
C	CALL USPEC(N,MATNO)	LEV02640
C		LEV02650
C	WHERE N IS THE ORDER OF THE USER-SUPPLIED MATRIX A, AND	LEV02660
C	MATNO IS A $\leq 8$ DIGIT INTEGER USED AS A MATRIX AND	LEV02670
C	TEST IDENTIFICATION NUMBER. IN ALL CASES THIS (THESE)	LEV02680
C	SUBROUTINE(S) DEFINES (DIMENSIONS) THE ARRAYS REQUIRED	LEV02690
C	TO SPECIFY THE MATRIX (MATRICES IN CASE (4)) THAT WILL BE	LEV02700
C	USED BY THE LANCZS SUBROUTINE. IN CASES (1) AND (2)	LEV02710

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C THIS IS THE A-MATRIX; IN CASE (3) THIS IS THE FACTORIZATION      LEV02720
C OF A SCALED, SHIFTED AND PERMUTED VERSION OF THE                LEV02730
C USER-SPECIFIED A-MATRIX. IN CASE (4) THE A-MATRIX              LEV02740
C IS SPECIFIED AS WELL AS THE FACTORIZATION OF THE                LEV02750
C B-MATRIX. THIS SUBROUTINE ALSO INITIALIZES THE ARRAYS          LEV02760
C AND ANY OTHER PARAMETERS NEEDED TO DEFINE THE MATRIX           LEV02770
C (MATRICES). THE STORAGE LOCATIONS OF THESE PARAMETERS          LEV02780
C AND ARRAYS ARE THEN PASSED TO THE MATRIX-VECTOR MULTIPLY       LEV02790
C SUBROUTINE CMATV IN CASES (1) AND (2), TO THE SUBROUTINE        LEV02800
C BSOLV IN CASE (3), AND TO THE SUBROUTINES AMATV                 LEV02810
C AND LSOLV IN CASE (4) VIA ENTRY CALLS. IN CASES (3) AND (4)    LEV02820
C WHENEVER A MATRIX HAS BEEN PERMUTED, THERE IS ALSO AN         LEV02830
C ENTRY INTO THE SUBROUTINE LPERM TO PASS THE LOCATIONS OF       LEV02840
C THE PERMUTATIONS IPR AND IPRT USED. SAMPLE USPECS, CMATV,      LEV02850
C AMATV, BSOLV AND LSOLV SUBROUTINES ARE INCLUDED               LEV02860
C IN THE RELEVANT FILES. THESE SAMPLE PROGRAMS ASSUME THAT       LEV02870
C THE USER-SUPPLIED A-MATRIX IS STORED ON FILE 8 IN CASES (1),   LEV02880
C (2), AND (4), AND THAT THE FACTORIZATION OF THE B-MATRIX       LEV02890
C IS ON FILE 7 IN CASES (3) AND (4). THE USER SHOULD SEE        LEV02900
C THE INDIVIDUAL SAMPLE SUBROUTINES FOR MORE DETAILS.           LEV02910
C                                                                    LEV02920
C IN CASES (1) AND (2):                                          LEV02930
C SUBROUTINE CMATV HAS THE CALLING SEQUENCE                       LEV02940
C                                                                    LEV02950
C     CALL CMATV(W,U,SUM)                                         LEV02960
C                                                                    LEV02970
C IN THE REAL SYMMETRIC CASE, U AND W ARE REAL*8 VECTORS         LEV02980
C AND SUM IS A REAL*8 SCALAR. IN THE HERMITIAN CASE, U           LEV02990
C AND W ARE COMPLEX*16 VECTORS AND SUM IS A REAL*8 SCALAR.      LEV03000
C CMATV CALCULATES  $U = A*W - SUM*U$  FOR THE USER-SPECIFIED      LEV03010
C MATRIX A. ONE OF THE SAMPLE CMATV SUBROUTINES INCLUDED         LEV03020
C COMPUTES MATRIX-VECTOR MULTIPLIES FOR AN ARBITRARY SPARSE,    LEV03030
C SYMMETRIC MATRIX STORED IN THE SPARSE FORMAT SPECIFIED IN THE LEV03040
C CORRESPONDING SAMPLE USPEC SUBROUTINE. FOR CASES (1) AND      LEV03050
C (2) CMATV IS THE SUBROUTINE USED BY THE LANCZS SUBROUTINE     LEV03060
C THAT GENERATES THE T-MATRICES. IN CASE (4) SUBROUTINE         LEV03070
C AMATV HAS THE SAME CALLING SEQUENCE AS CMATV IN CASE (1).     LEV03080
C                                                                    LEV03090
C IN CASES (3) AND (4):                                          LEV03100
C ALPHA/BETA HISTORY IS GENERATED USING SPARSE MATRIX INVERSION. LEV03110
C IN CASE (3), AT EACH ITERATION OF THE LANCZOS RECURSION      LEV03120
C GIVEN A FACTORIZATION OF THE MATRIX BEING USED, THE           LEV03130
C SUBROUTINE BSOLV FOR A GIVEN V, COMPUTES U SUCH THAT  $B*U = V$ . LEV03140
C THE CALLING SEQUENCE OF BSOLV IS                               LEV03150
C                                                                    LEV03160
C     CALL BSOLV(V,U,IBSOLV)                                     LEV03170
C                                                                    LEV03180
C WHEN IBSOLV = 2,  $U = (B-INVESRE)*V$  IS RETURNED. IN CASE (4), LEV03190
C AT EACH ITERATION OF THE GENERALIZED LANCZOS RECURSION BOTH THE LEV03200
C SUBROUTINE AMATV AND THE SUBROUTINE LSOLV ARE USED. THE       LEV03210
C CALLING SEQUENCE OF LSOLV IS                                   LEV03220
C                                                                    LEV03230
C     CALL LSOLV(V,U,ISOLV)                                       LEV03240
C                                                                    LEV03250
C WHERE U AND V ARE REAL*8 VECTORS. LSOLV PERFORMS 4 FUNCTIONS. LEV03260

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C   LET L DENOTE THE CHOLESKY FACTOR OF THE B-MATRIX USED IN LANCZS.   LEV03270
C   WHEN ISOLV = 1, LSOLV COMPUTES  $U = L*V$ .   WHEN ISOLV = 2,   LEV03280
C   LSOLV COMPUTES  $U = (L-TRANSPOSE)*V$ .   WHEN ISOLV = 3, LSOLV   LEV03290
C   COMPUTES  $U = (L-INVERSE)*V$ .   WHEN ISOLV = 4, LSOLV   LEV03300
C   COMPUTES  $U = ((L-TRANSPOSE)-INVERSE)*V$ .   LEV03310
C   LEV03320
C   SAMPLE PROGRAMS ASSUME THAT THE A-MATRIX (CASES (1),(2),(4))   LEV03330
C   IS ON FILE 8 AND STORED IN THE FOLLOWING SPARSE FORMAT:   LEV03340
C   ICOL(K), K = 1,NZL, NUMBER OF SUBDIAGONAL NONZEROS IN COLUMN K.   LEV03350
C   IROW(K), K = 1,NZS, ROW INDEX OF ASD(K).   LEV03360
C   AD(K), K=1,N, CONTAINS THE DIAGONAL ELEMENTS OF THE A-MATRIX.   LEV03370
C   ASD(K), K=1,NZS CONTAINS THE SUBDIAGONAL ELEMENTS OF A BY COLUMN. LEV03380
C   NZS = NUMBER OF NONZERO ELEMENTS BELOW THE DIAGONAL OF A   LEV03390
C   NZL = INDEX OF LAST COLUMN WITH NONZERO SUBDIAGONAL ENTRIES   LEV03400
C   N = ORDER OF THE A-MATRIX.   LEV03410
C   LEV03420
C   NOTE THAT THE OPTIONAL PREPROCESSING PROGRAMS PERMUT AND   LEV03430
C   LORDER ASSUME THAT THE GIVEN MATRIX IS ON FILE 8.   CASES (3)   LEV03440
C   AND (4) ASSUME THAT THE SPARSE FACTORIZATION OF B IS STORED ON   LEV03450
C   FILE 7.   THE SAMPLE BSOLV SUBROUTINE SUPPLIED ASSUMES   LEV03460
C   THAT THE B-MATRIX IS POSITIVE DEFINITE AND THAT ITS CHOLESKY   LEV03470
C   FACTOR IS PROVIDED ON FILE 7, STORED IN SPARSE FORMAT IN   LEV03480
C   ARRAYS BD AND BSD.   THE USER CAN EASILY REPLACE THIS SAMPLE   LEV03490
C   BSOLV SUBROUTINE AND THE CORRESPONDING SAMPLE USPEC   LEV03500
C   SUBROUTINE BY SUBROUTINES THAT DEFINE AND USE A GENERAL   LEV03510
C   FACTORIZATION  $L*D*(L-TRANSPOSE)$ .   LEV03520
C   LEV03530
C   THE SAMPLE USPEC, CMATV (CASES (1) AND (2)), AMATV (CASE (4)),   LEV03540
C   BSOLV (CASE (3)), AND LSOLV (CASE(4)) MUST BE MODIFIED BY   LEV03550
C   THE USER TO ACCOMODATE THE USER-SPECIFIED MATRIX OR MATRICES.   LEV03560
C   LEV03570
C   LEV03580
C-----MACHEP-----LEV03590
C   LEV03600
C   LEV03610
C   MACHEP IS A MACHINE DEPENDENT PARAMETER SPECIFYING THE RELATIVE   LEV03620
C   PRECISION OF THE FLOATING POINT ARITHMETIC USED.   LEV03630
C   MACHEP =  $2.2 * 10^{*-16}$  FOR DOUBLE PRECISION ARITHMETIC ON   LEV03640
C   IBM 370-3081.   LEV03650
C   LEV03660
C   THE USER WILL HAVE TO RESET THIS PARAMETER TO   LEV03670
C   THE CORRESPONDING VALUE FOR THE MACHINE BEING USED.   NOTE THAT   LEV03680
C   IF A MACHINE WITH A MACHINE EPSILON THAT IS MUCH LARGER THAN THE   LEV03690
C   VALUE GIVEN HERE IS BEING USED, THEN THERE COULD BE   LEV03700
C   PROBLEMS WITH THE TOLERANCES.   LEV03710
C   LEV03720
C   LEV03730
C-----SUBROUTINES AND FUNCTIONS USER MUST SUPPLY-----LEV03740
C   LEV03750
C   LEV03760
C   GENRAN, FINPRO, MASK, USPEC, AND   LEV03770
C   CASES (1) AND (2), CMATV: CASE (3), BSOLV:   LEV03780
C   CASE (4), AMATV AND LSOLV.   LEV03790
C   LEV03800
C   GENRAN = COMPUTES K PSEUDO-RANDOM NUMBERS AND STORES THEM IN   LEV03810

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C-----LEVO4370
C                                         LEVO4380
C                                         LEVO4390
C-----PARAMETER CONTROLS FOR EIGENVALUE PROGRAMS-----LEVO4400
C                                         LEVO4410
C                                         LEVO4420
C   PARAMETER CONTROLS ARE INTRODUCED TO ALLOW SEGMENTATION OF THE LEVO4430
C   EIGENVALUE COMPUTATIONS AND TO ALLOW VARIOUS COMBINATIONS OF LEVO4440
C   READ/WRITES. LEVO4450
C                                         LEVO4460
C   THE FLAG ISTART CONTROLS THE T-MATRIX (ALPHA/BETA HISTORY) LEVO4470
C   GENERATION. LEVO4480
C                                         LEVO4490
C   ISTART = (0,1) MEANS LEVO4500
C                                         LEVO4510
C       (0) THERE IS NO EXISTING ALPHA/BETA HISTORY AND ONE LEVO4520
C           MUST BE GENERATED. LEVO4530
C                                         LEVO4540
C       (1) THERE IS AN EXISTING ALPHA/BETA HISTORY AND IT IS LEVO4550
C           TO BE READ IN FROM FILE 2 AND EXTENDED IF NECESSARY. LEVO4560
C                                         LEVO4570
C   THE FLAG ISTOP CAN BE USED IN CONJUNCTION WITH THE FLAG ISTART TO LEVO4580
C   ALLOW SEGMENTATION OF THE EIGENVALUE COMPUTATIONS. LEVO4590
C                                         LEVO4600
C   ISTOP = (0,1) MEANS LEVO4610
C                                         LEVO4620
C       (0) PROGRAM COMPUTES ONLY THE REQUESTED ALPHAS/BETAS, LEVO4630
C           STORES THEM AND THE LAST 2 LANCZOS VECTORS GENERATED LEVO4640
C           IN FILE 1 AND THEN TERMINATES. IN CASE (4) THERE LEVO4650
C           ARE ACTUALLY 3 VECTORS TO BE SAVED. LEVO4660
C                                         LEVO4670
C       (1) PROGRAM COMPUTES REQUESTED ALPHAS/BETAS AND THEN LEVO4680
C           USES THE BISEC SUBROUTINE TO CALCULATE EIGENVALUES LEVO4690
C           OF THE TRIDIAGONAL MATRICES GENERATED FOR THE ORDERS LEVO4700
C           SPECIFIED BY THE USER AND ON THE USER-SPECIFIED LEVO4710
C           INTERVALS. PROGRAM THEN USES THE SUBROUTINE INVERR LEVO4720
C           TO COMPUTE ERROR ESTIMATES FOR THE ISOLATED GOOD LEVO4730
C           T-EIGENVALUES WHICH ARE USED TO CHECK THE LEVO4740
C           CONVERGENCE OF THESE T-EIGENVALUES. LEVO4750
C                                         LEVO4760
C   CONTROL PARAMETERS FOR WRITES LEVO4770
C                                         LEVO4780
C   ITHIS = (0,1) MEANS LEVO4790
C                                         LEVO4800
C       (0) IF ISTOP .GT. 0 THEN ALPHA/BETAS ARE NOT SAVED ON LEVO4810
C           FILE 1. LEVO4820
C                                         LEVO4830
C       (1) PROGRAM WRITES ALPHAS/BETAS AND LAST 2 LANCZOS LEVO4840
C           VECTORS TO FILE 1 SO THAT THE T-MATRIX GENERATION LEVO4850
C           MAY BE REUSED OR CONTINUED LATER IF NECESSARY. LEVO4860
C           TYPICALLY ONE WOULD ALWAYS DO THIS ON ANY RUN WHERE LEVO4870
C           A HISTORY FILE IS BEING GENERATED. HISTORY MUST BE LEVO4880
C           SAVED IN MACHINE FORMAT ((4Z20) FOR IBM 3081) SO LEVO4890
C           THAT NO ERRORS ARE INTRODUCED BY FORMAT CONVERSIONS. LEVO4900
C                                         LEVO4910

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C   IDIST = (0,1)  MEANS                                LEV04920
C                                                       LEV04930
C           (0) DISTINCT EIGENVALUES OF T-MATRICES ARE NOT SAVED. LEV04940
C                                                       LEV04950
C           (1) PROGRAM WRITES COMPUTED DISTINCT EIGENVALUES OF LEV04960
C               T-MATRICES ALONG WITH THEIR T-MULTIPLICITIES LEV04970
C               TO FILE 11.                                LEV04980
C                                                       LEV04990
C   IWRITE = (0,1)  MEANS                                LEV05000
C                                                       LEV05010
C           (0) NO EXTENDED OUTPUT FROM SUBROUTINES BISEC AND INVERR LEV05020
C               IS SENT TO FILE 6.                        LEV05030
C                                                       LEV05040
C           (1) INDIVIDUAL COMPUTED T-EIGENVALUES AND CORRESPONDING LEV05050
C               ERROR ESTIMATES FROM THE SUBROUTINES BISEC AND INVERR LEV05060
C               ARE PRINTED OUT TO FILE 6 AS THEY ARE COMPUTED. LEV05070
C                                                       LEV05080
C   THE PROGRAM ALWAYS MAKES A SEPARATE LIST OF THE COMPUTED GOOD LEV05090
C   T-EIGENVALUES ALONG WITH THEIR MINIMAL GAPS AND WRITES THEM OUT LEV05100
C   TO FILE 3.  CORRESPONDING ERROR ESTIMATES FOR ANY ISOLATED LEV05110
C   GOOD T-EIGENVALUES ARE ALWAYS WRITTEN TO FILE 4.     LEV05120
C                                                       LEV05130
C                                                       LEV05140
C-----INPUT/OUTPUT FILES FOR EIGENVALUE PROGRAMS-----LEV05150
C                                                       LEV05160
C   ANY INPUT DATA OTHER THAN THE ALPHA/BETA HISTORY SHOULD BE STORED LEV05170
C   ON FILE 5.  SEE SAMPLE INPUT/OUTPUT FROM TYPICAL RUN. LEV05180
C   THE READ STATEMENTS IN THE GIVEN FORTRAN PROGRAM ASSUME THAT LEV05190
C   THE DATA STORED ON FILE 5 IS IN FREE FORMAT.  USER SHOULD NOTE LEV05200
C   THAT 'FREE FORMAT' IS NOT CLASSIFIED AS PORTABLE BY PFORT SO THAT LEV05210
C   THE USER MAY HAVE TO MODIFY THE READ STATEMENTS FROM FILE 5 TO LEV05220
C   CONFORM TO WHAT IS PERMISSIBLE ON THE MACHINE BEING USED. LEV05230
C                                                       LEV05240
C   FILE 6 WAS USED AS THE INTERACTIVE TERMINAL OUTPUT FILE. LEV05250
C   THIS FILE PROVIDES A RUNNING ACCOUNT OF THE PROGRESS OF THE LEV05260
C   COMPUTATIONS.  THE AMOUNT OF INFORMATION PRINTED OUT IS LEV05270
C   CONTROLLED BY THE PARAMETER IWRITE.                  LEV05280
C                                                       LEV05290
C DESCRIPTION OF OTHER I/O FILES                          LEV05300
C                                                       LEV05310
C FILE (K)   CONTAINS:                                    LEV05320
C                                                       LEV05330
C   (1)      OUTPUT FILE:                                  LEV05340
C           HISTORY FILE OF NEWLY-GENERATED T-MATRIX (ALPHA AND LEV05350
C           BETA VECTORS) AND LAST 2 LANCZOS VECTORS USED LEV05360
C           IN THE T-MATRIX GENERATION.  NOTE THAT IN CASE (4) LEV05370
C           THREE 'LANCZOS' VECTORS ARE WRITTEN TO FILE 1. LEV05380
C           IF ITHIS = 0 AND ISTOP = 1, FILE 1 IS NOT WRITTEN. LEV05390
C                                                       LEV05400
C   (2)      INPUT FILE:                                   LEV05410
C           SAME AS FILE 1 EXCEPT THAT IT CONTAINS A LEV05420
C           PREVIOUSLY-GENERATED T-MATRIX (IF ANY).  IF ISTART = 1, LEV05430
C           PROGRAM ASSUMES THAT THERE IS A HISTORY FILE OF ALPHAS LEV05440
C           AND BETAS ON FILE 2.  THESE ALPHAS AND BETAS ARE LEV05450
C           READ IN ALONG WITH THE LAST 2 LANCZOS VECTORS THAT LEV05460

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C          WERE GENERATED.  IN CASE (4) THREE 'LANCZOS' VECTORS      LEV05470
C          ARE READ IN FROM FILE 2.                                  LEV05480
C                                                                    LEV05490
C  (3)     OUTPUT FILE:                                           LEV05500
C          COMPUTED GOOD EIGENVALUES OF THE T-MATRICES USED. ALSO  LEV05510
C          CONTAINS T-MULTIPLICITIES OF THESE EIGENVALUES AS      LEV05520
C          EIGENVALUES OF THE T-MATRIX, AND THEIR GAPS AS        LEV05530
C          EIGENVALUES IN THE A-MATRIX AND IN THE T-MATRIX.      LEV05540
C          FILE 3 IS ALWAYS WRITTEN.  IN CASE (3) THIS OUTPUT    LEV05550
C          CONTAINS THE EIGENVALUES OF THE B-INVERSE MATRIX      LEV05560
C          SINCE IN THIS CASE THE T-MATRICES CORRESPOND TO      LEV05570
C          THE B-INVERSE MATRIX AND NOT TO THE A-MATRIX.  IN    LEV05580
C          THIS CASE, 3 SETS OF GAPS ARE GIVEN, THOSE IN        LEV05590
C          THE T-MATRIX, IN THE B-INVERSE MATRIX AND THOSE      LEV05600
C          FOR THE CORRESPONDING EIGENVALUES IN THE A-MATRIX.    LEV05610
C                                                                    LEV05620
C  (4)     OUTPUT FILE:                                           LEV05630
C          ERROR ESTIMATES FOR THE ISOLATED GOOD T-EIGENVALUES  LEV05640
C          WHICH ARE OBTAINED USING THE SUBROUTINE INVERR. THESE LEV05650
C          ESTIMATES USE THE LAST COMPONENTS OF THE ASSOCIATED  LEV05660
C          T-EIGENVECTORS WHICH ARE COMPUTED USING INVERSE      LEV05670
C          ITERATION.  FILE 4 IS ALWAYS WRITTEN.                LEV05680
C                                                                    LEV05690
C                                                                    LEV05700
C  (7)     INPUT FILE:                                           LEV05710
C          USED ONLY IN CASES (3) AND (4), FACTORED INVERSES    LEV05720
C          OF REAL SYMMETRIC MATRICES AND GENERALIZED EIGENVALUE LEV05730
C          PROBLEM.  CONTAINS THE REQUIRED FACTORIZATION OF THE   LEV05740
C          B-MATRIX.                                           LEV05750
C                                                                    LEV05760
C  (8)     INPUT FILE:                                           LEV05770
C          SAMPLE USPEC SUBROUTINE ASSUMES THAT THE ARRAYS      LEV05780
C          REQUIRED TO SPECIFY THE USER'S-MATRIX ARE STORED ON   LEV05790
C          FILE 8.  USERS MUST MAKE WHATEVER DEFINITIONS ARE    LEV05800
C          APPROPRIATE FOR THEIR MATRICES.  NOTE THAT IN CASE  LEV05810
C          (3) THE LANCZS SUBROUTINE DOES NOT USE THE MATRIX     LEV05820
C          ON FILE 8 IN THE T-MATRIX GENERATION, RATHER IT      LEV05830
C          USES THE FACTORIZATION OF AN ASSOCIATED               LEV05840
C          B-MATRIX WHICH IS STORED ON FILE 7.  IN CASE (4),    LEV05850
C          THE INFORMATION STORED ON BOTH FILES 7 AND 8 IS USED. LEV05860
C                                                                    LEV05870
C  (9)     INPUT AND OUTPUT FILE:                                 LEV05880
C          CAN BE USED TO STORE THE TRUE EIGENVALUES OF THE    LEV05890
C          GIVEN PROBLEM, WHEN THE PROCEDURE                    LEV05900
C          IS BEING EXERCISED ON A TEST MATRIX.                LEV05910
C                                                                    LEV05920
C  (11)    OUTPUT FILE:                                          LEV05930
C          COMPUTED DISTINCT EIGENVALUES OF T-MATRICES USED.   LEV05940
C          ALSO CONTAINS THEIR T-MULTIPLICITIES AND T-GAPS TO   LEV05950
C          NEAREST DISTINCT EIGENVALUES, AND THE T-MULTIPLICITY LEV05960
C          PATTERN OF THE GOOD AND THE SPURIOUS T-EIGENVALUES. LEV05970
C          FILE 11 IS WRITTEN ONLY IF IDIST = 1.                LEV05980
C                                                                    LEV05990
C                                                                    LEV06000
C-----PARAMETERS SET BY THE EIGENVALUE PROGRAMS----- LEV06010

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C                                                    LEV06020
C                                                    LEV06030
C THESE PARAMETERS ARE SET INTERNALLY IN THE PROGRAM LEV06040
C                                                    LEV06050
C SCALEK      K = 1,2,3,4                            LEV06060
C                                                    LEV06070
C           THE SCALING FACTORS SCALEK HAVE BEEN INTRODUCED IN AN LEV06080
C           ATTEMPT TO MAKE THE TOLERANCES USED IN THE           LEV06090
C           T-MULTIPLICITY, SPURIOUS, ISOLATION AND PRTESTS ADJUST LEV06100
C           TO THE SCALE OF THE GIVEN MATRIX.  THESE FACTORS MUST LEV06110
C           NOT BE MODIFIED.  THESE TOLERANCES OCCUR IN LUMP,     LEV06120
C           ISOEV, AND PRTEST.                                    LEV06130
C                                                    LEV06140
C NOTE:      THE USER SHOULD NOTE THAT IF THE MATRIX BEING     LEV06150
C           PROCESSED IS VERY STIFF, THAT IS THE RATIO OF THE LARGEST LEV06160
C           EIGENVALUE IN MAGNITUDE TO THE SMALLEST IN MAGNITUDE IS VERY LEV06170
C           LARGE, THEN THE TOLERANCES BEING USED IN BISEC, LUMP, ISOEV LEV06180
C           AND PRTEST MAY NOT TREAT THE SMALL END (SMALL IN MAGNITUDE) LEV06190
C           VERY WELL.  IN SOME SUCH CASES A USER-INTRODUCED REDUCTION LEV06200
C           IN THE SIZE OF TKMAX AND THE SUBSEQUENT RECOMPUTATION OF LEV06210
C           THE T-MATRIX EIGENVALUES IN (ONLY) THE LOWER END OF THE LEV06220
C           SPECTRUM WITH THIS TKMAX MAY RESULT IN IMPROVED COMPUTATIONS LEV06230
C           AT THE LOW END.                                       LEV06240
C                                                    LEV06250
C           THE LUMP, ISOEV, AND PRTEST TOLERANCES THAT WERE USED LEV06260
C           MOST IN THE TESTING OF THESE ALGORITHMS WERE NOT      LEV06270
C           SCALE INVARIANT BUT SEEMED TO WORK WELL ON MATRICES THAT LEV06280
C           HAD EIGENVALUES WITH MAGNITUDES BOTH GREATER THAN AND LESS LEV06290
C           THAN 1.  THESE TOLERANCES ARE ALSO INCLUDED IN THESE THREE LEV06300
C           SUBROUTINES BUT AS COMMENTED OUT STATEMENTS.  THEY CAN BE LEV06310
C           REVIVED BY COMMENTING OUT THE CORRESPONDING TOLERANCES LEV06320
C           SPECIFIED IN THE STATEMENT ABOVE EACH OF THESE.      LEV06330
C                                                    LEV06340
C           IMPORTANT TOLERANCES OR SCALES THAT ARE USED REPEATEDLY LEV06350
C           THROUGHOUT THE LANCZOS EIGENVALUE PROGRAMS ARE THE FOLLOWING: LEV06360
C           SCALED MACHINE EPSILON:  TTOL = TKMAX*EPSM WHERE      LEV06370
C           EPSM = 2*MACHINE EPSILON AND                          LEV06380
C           TKMAX = MAX(|ALPHA(J)|, BETA(J), J = 1, MEV)           LEV06390
C           BISEC CONVERGENCE TOLERANCE:  BISTOL = DSQRT(1000+MEV)*TTOL LEV06400
C           BISEC T-MULTIPLICITY TOLERANCE:  MULTOL = (1000+MEV)*TTOL LEV06410
C           LANCZOS CONVERGENCE TOLERANCE:  CONTOL = BETA(MEV+1)*1.D-10 LEV06420
C                                                    LEV06430
C                                                    LEV06440
C           BTOL = RELATIVE TOLERANCE USED TO ESTIMATE ANY LOSS OF LOCAL LEV06450
C           ORTHOGONALITY OF THE LANCZOS VECTORS AFTER THE T-MATRIX LEV06460
C           HAS BEEN GENERATED.  THE LANCZOS PROCEDURE WORKS WELL LEV06470
C           ONLY IF LOCAL ORTHOGONALITY BETWEEN SUCCESSIVE LANCZOS LEV06480
C           VECTORS IS MAINTAINED.  THE TNORM SUBROUTINE TESTS LEV06490
C           WHETHER OR NOT                                       LEV06500
C                                                    LEV06510
C           MINIMUM |BETA(I)|/||A|| > BTOL.                       LEV06520
C           I=2,KMAX                                              LEV06530
C                                                    LEV06540
C           IF THIS TEST IS VIOLATED BY SOME BETA AND A T-MATRIX THAT LEV06550
C           WOULD INCLUDE SUCH A BETA IS REQUESTED, THEN THE LANCZOS LEV06560

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C          PROCEDURE WILL TERMINATE FOR THE USER TO DECIDE WHAT TO   LEV06570
C          DO.  THE USER CAN OVER-RIDE THIS TEST BY SIMPLY DECREASING LEV06580
C          THE SIZE OF BTOL, BUT THEN CONVERGENCE IS NOT AS CERTAIN.  LEV06590
C          THE PROGRAM SETS BTOL = 1.D-8 WHICH IS A VERY CONSERVATIVE LEV06600
C          CHOICE.  THE || A || IS ESTIMATED BY USING AN ESTIMATE     LEV06610
C          OF THE NORM OF THE T-MATRIX, T(1,KMAX).                    LEV06620
C                                                                      LEV06630
C          GAPTOL = RELATIVE TOLERANCE USED IN THE SUBROUTINE ISOEV   LEV06640
C          TO DETERMINE WHICH OF THE GOOD T-EIGENVALUES NEED        LEV06650
C          ERROR ESTIMATES.  THE PROGRAM SETS GAPTOL = 1.D-8.      LEV06660
C          IF FOR A GIVEN 'GOOD' T-EIGENVALUE THE COMPUTED GAP      LEV06670
C          IS TOO SMALL AND IS DUE TO A 'SPURIOUS' T-EIGENVALUE    LEV06680
C          THEN THE 'GOOD' T-EIGENVALUE IS ASSUMED TO HAVE CONVERGED LEV06690
C          AND NO ERROR ESTIMATES ARE COMPUTED.                     LEV06700
C                                                                      LEV06710
C                                                                      LEV06720
C-----USER-SPECIFIED PARAMETERS FOR EIGENVALUE PROGRAMS----- LEV06730
C                                                                      LEV06740
C                                                                      LEV06750
C          RELTOL = RELATIVE TOLERANCE USED IN 'COMBINING' COMPUTED LEV06760
C          EIGENVALUES OF T(1,MEV) PRIOR TO COMPUTING ERROR        LEV06770
C          ESTIMATES.                                              LEV06780
C                                                                      LEV06790
C          THE LUMPING OF T-EIGENVALUES OCCURS IN SUBROUTINE LUMP.  LEV06800
C          LUMPING IS NECESSARY BECAUSE IT IS IMPOSSIBLE TO ACCURATELY LEV06810
C          PREDICT THE ACCURACY OF THE BISEC SUBROUTINE.  LUMP 'COMBINES' LEV06820
C          T-EIGENVALUES THAT HAVE SLIPPED BY THE TOLERANCE THAT WAS USED LEV06830
C          IN THE T-MULTIPLICITY TESTS.  IN PARTICULAR IF FOR SOME J, LEV06840
C          |EVALUE(J)-EVALUE(J-1)| < DMAX1(RELTOL*|EVALUE(J)|,SCALE2*MULTOL) LEV06860
C          THEN THESE T-EIGENVALUES ARE 'COMBINED'.  MULTOL IS THE TOLERANCE LEV06880
C          THAT WAS USED IN THE T-MULTIPLICITY TEST IN BISEC.  SEE THE HEADER LEV06890
C          ON THE LUMP SUBROUTINE FOR MORE DETAILS.                 LEV06900
C                                                                      LEV06910
C          RELTOL IS SET TO 1.D-10.                                LEV06920
C                                                                      LEV06930
C          MXINIT = MAXIMUM NUMBER OF INVERSE ITERATIONS ALLOWED IN LEV06940
C          SUBROUTINE INVERR FOR EACH ISOLATED GOOD T-EIGENVALUE.  LEV06950
C          TYPICALLY ONLY ONE ITERATION IS REQUIRED.                LEV06960
C                                                                      LEV06970
C          SEEDS FOR RANDOM NUMBER GENERATORS = INTEGER*4 SCALARS. LEV06980
C                                                                      LEV06990
C          (1) SVSEED = SEED FOR STARTING VECTOR USED IN          LEV07000
C          T-MATRIX GENERATION IN LANCZS SUBROUTINE                LEV07010
C                                                                      LEV07020
C          (2) RHSEED = SEED FOR RIGHT-HAND SIDE USED IN          LEV07030
C          INVERSE ITERATION COMPUTATIONS IN INVERR.              LEV07040
C                                                                      LEV07050
C          BISEC DATA                                             LEV07060
C                                                                      LEV07070
C          (1) NINT = NUMBER OF SUBINTERVALS ON WHICH EIGENVALUES ARE LEV07080
C          TO BE COMPUTED.                                         LEV07090
C                                                                      LEV07100
C          (2) LB(J) = (J = 1,NINT) = LEFT END POINTS OF THESE INTERVALS. LEV07110

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C          MUST BE PROVIDED IN INCREASING ORDER.  THAT IS,      LEV07120
C          LB(J) < LB(J+1) FOR J = 1,NINT.                        LEV07130
C                                                                LEV07140
C      (3) UB(J) = (J = 1,NINT) = RIGHT END POINTS OF THESE INTERVALS. LEV07150
C          MUST BE PROVIDED IN INCREASING ORDER.  THAT IS,      LEV07160
C          UB(J) < UB(J+1) FOR J = 1,NINT.                        LEV07170
C                                                                LEV07180
C      (4) MXSTUR = MAXIMUM NUMBER OF STURM ITERATIONS ALLOWED FOR LEV07190
C          ENTIRE SET OF EIGENVALUE CALCULATIONS OVER ALL      LEV07200
C          SPECIFIED SIZE T-MATRICES.  PROGRAM WILL            LEV07210
C          TERMINATE IF THIS LIMIT IS EXCEEDED.                LEV07220
C                                                                LEV07230
C      T-MATRICES                                              LEV07240
C                                                                LEV07250
C      SIZES OF T-MATRICES                                    LEV07260
C                                                                LEV07270
C          (1) KMAX= MAXIMUM ORDER FOR T-MATRIX THAT USER IS WILLING LEV07280
C              TO CONSIDER.                                    LEV07290
C                                                                LEV07300
C          (2) NMEVS = MAXIMUM NUMBER OF T-MATRICES THAT WILL BE LEV07310
C              CONSIDERED.                                    LEV07320
C                                                                LEV07330
C          (3) NMEV(J) (J=1,NMEVS) = SIZES OF T-MATRIX TO BE LEV07340
C              CONSIDERED SEQUENTIALLY.                      LEV07350
C                                                                LEV07360
C      T-MATRIX-GENERATION                                    LEV07370
C                                                                LEV07380
C      USER SHOULD NOTE THAT THIS PROGRAM FIRST COMPUTES A T-MATRIX LEV07390
C      OF ORDER KMAX AND THEN CYCLES THROUGH THE T-MATRICES SPECIFIED LEV07400
C      A PRIORI BY THE USER, USING THE SUBROUTINE BISEC TO COMPUTE THE LEV07410
C      EIGENVALUES OF THE T-MATRICES ON THE INTERVALS SPECIFIED BY LEV07420
C      THE USER.                                             LEV07430
C                                                                LEV07440
C      IDEALLY, ONE WOULD COMPUTE THE EIGENVALUE APPROXIMATIONS AT A LEV07450
C      REASONABLE SIZE T-MATRIX, LOOK AT THE ACCURACY OF THE COMPUTED LEV07460
C      RESULTS AND USE THAT TO DETERMINE AN APPROPRIATE LEV07470
C      INCREMENT FOR THE SIZE OF THE T-MATRIX BASED UPON WHAT LEV07480
C      HAS ALREADY CONVERGED AND UPON THE SIZES OF THE ERROR ESTIMATES LEV07490
C      ON THOSE EIGENVALUES THAT ARE DESIRED BUT THAT HAVE NOT YET LEV07500
C      CONVERGED. HOWEVER, IN THE INTERESTS OF GENERALITY AND LEV07510
C      SIMPLICITY WE DID NOT DO THAT HERE.                  LEV07520
C                                                                LEV07530
C                                                                LEV07540
C-----CONVERGENCE TESTS FOR THE EIGENVALUE PROGRAMS----- LEV07550
C                                                                LEV07560
C                                                                LEV07570
C      THE CONVERGENCE TEST INCORPORATED IN THIS PROGRAM IS LEV07580
C      BASED UPON THE ASSUMPTION THAT THOSE T-EIGENVALUES AND THEIR LEV07590
C      ASSOCIATED T-EIGENVECTORS WHICH CORRESPOND TO THE LEV07600
C      EIGENVALUES AND RITZVECTORS WHICH WE WISH TO COMPUTE LEV07610
C      CONVERGE AS THE T-SIZE IS INCREASED.                 LEV07620
C                                                                LEV07630
C      AS CURRENTLY PROGRAMMED, CONVERGENCE IS CHECKED BY EXAMINING LEV07640
C      THE SIZES OF ALL OF THE COMPUTED ERROR ESTIMATES ON ALL OF THE LEV07650
C      INTERVALS SPECIFIED BY THE USER.  IDEALLY CONVERGENCE SHOULD LEV07660

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C      BE CHECKED ONLY ON THOSE EIGENVALUES OF INTEREST AND          LEV07670
C      ONCE THE EIGENVALUES ON SUB-INTERVALS OF THESE INTERVALS HAVE  LEV07680
C      CONVERGED, ANY SUBSEQUENT EIGENVALUE COMPUTATIONS SHOULD BE   LEV07690
C      MADE ONLY ON THE UNCONVERGED PORTIONS.  OBVIOUSLY, IT WOULD BE LEV07700
C      DIFFICULT TO INCORPORATE CODE TO DO THE ABOVE WITHOUT KNOWING  LEV07710
C      A PRIORI PRECISELY WHAT THE USER IS TRYING TO COMPUTE.        LEV07720
C      THEREFORE, WE DID NOT ATTEMPT TO DO THIS.  IF ONE WISHES TO   LEV07730
C      MAKE SUCH A MODIFICATION THEN ONE MUST ALSO MODIFY THE PROGRAM  LEV07740
C      SO THAT IT CREATES AN OVERALL LIST OF THE CONVERGED 'GOOD'     LEV07750
C      T-EIGENVALUES AS THEY ARE COMPUTED, SINCE CONVERGED 'GOOD'    LEV07760
C      T-EIGENVALUES WHICH WERE COMPUTED AT A PARTICULAR VALUE OF MEV LEV07770
C      WOULD NO LONGER BE RECOMPUTED AT LARGER VALUES OF MEV.       LEV07780
C                                                                    LEV07790
C      IF ONLY A FEW EIGENVALUES ARE TO BE COMPUTED THEN SUCH CHANGES LEV07800
C      WOULD NOT MAKE MUCH DIFFERENCE IN THE RUNNING TIME.          LEV07810
C                                                                    LEV07820
C                                                                    LEV07830
C-----ARRAYS REQUIRED BY THE EIGENVALUE PROGRAMS-----LEV07840
C                                                                    LEV07850
C                                                                    LEV07860
C      ALL 4 CASES                                                  LEV07870
C                                                                    LEV07880
C      ALPHA(J) = REAL*8 ARRAY.  ITS DIMENSION MUST BE AT LEAST KMAX, LEV07890
C      THE LENGTH OF THE LARGEST T-MATRIX ALLOWED.  THIS           LEV07900
C      ARRAY CONTAINS THE DIAGONAL ENTRIES OF THE T-MATRICES.      LEV07910
C                                                                    LEV07920
C      BETA(J) = REAL*8 ARRAY.  ITS DIMENSION MUST BE AT LEAST KMAX+1. LEV07930
C      THIS ARRAY CONTAINS THE SUBDIAGONAL ENTRIES OF THE         LEV07940
C      T-MATRICES.                                                 LEV07950
C                                                                    LEV07960
C      THE ALPHA AND BETA VECTORS ARE NOT ALTERED                  LEV07970
C      DURING THE CALCULATIONS.                                    LEV07980
C                                                                    LEV07990
C      V1(J),V2(J),VS(J) = REAL*8 ARRAYS IN REAL SYMMETRIC CASES.  LEV08000
C      V1 AND V2 ARE COMPLEX*16 IN HERMITIAN CASE.                LEV08010
C      IN CASES (1) AND (2) VS MUST BE OF                          LEV08020
C      DIMENSION AT LEAST KMAX.  IN CASES (3) AND                  LEV08030
C      (4) VS MUST BE OF DIMENSION AT LEAST                         LEV08040
C      MAX(N,KMAX).  IN REAL SYMMETRIC CASES                       LEV08050
C      V1 MUST BE OF DIMENSION AT LEAST                             LEV08060
C      MAX(KMAX+1,N) AND V2 MUST BE OF DIMENSION                   LEV08070
C      MAX(KMAX,N).  IN HERMITIAN CASES V1                         LEV08080
C      MUST BE OF DIMENSION MAX(N,(KMAX+1)/2)                      LEV08090
C      AND V2 OF DIMENSION AT LEAST MAX(N,KMAX/2).                 LEV08100
C      IN ALL CASES HOWEVER, THE ABOVE DIMENSIONS                  LEV08110
C      FOR V2 ARE VALID ONLY IF NO MORE                             LEV08120
C      THAN KMAX/2 EIGENVALUES OF THE GIVEN                        LEV08130
C      T-MATRICES ARE TO BE COMPUTED IN ANY GIVEN                 LEV08140
C      SUBINTERVAL.  V2 IS USED IN THE SUBROUTINE                  LEV08150
C      BISEC TO HOLD THE UPPER AND LOWER                           LEV08160
C      ENDPOINTS OF THE SUBINTERVALS GENERATED                    LEV08170
C      DURING THE BISECTIONS.  THEREFORE, ITS                      LEV08180
C      REAL*8 DIMENSION MUST ALWAYS BE AT LEAST                   LEV08190
C      2*Q WHERE Q IS THE MAXIMUM NUMBER OF                        LEV08200
C      EIGENVALUES OF THE SPECIFIED T-MATRIX IN ANY               LEV08210

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C ONE OF THE SPECIFIED INTERVALS. LEV08220  
 C NOTE THAT IN THE HERMITIAN CASE, V1 AND V2 LEV08230  
 C ARE DEFINED AS COMPLEX\*16 IN THE MAIN PROGRAM LEV08240  
 C AND IN THE LANCZS SUBROUTINE BUT ARE LEV08250  
 C REDEFINED AS REAL\*8 IN OTHER SUBROUTINES. LEV08260  
 C LEV08270  
 C LB(J),UB(J) = REAL\*8 ARRAYS. EACH MUST BE OF DIMENSION AT LEAST LEV08280  
 C NINT, THE NUMBER OF SUBINTERVALS TO BE CONSIDERED. LEV08290  
 C LB CONTAINS THE LEFT-END POINTS OF THE INTERVALS LEV08300  
 C ON WHICH EIGENVALUES ARE TO BE COMPUTED. UB LEV08310  
 C CONTAINS THE RIGHT-END POINTS. LEV08320  
 C LEV08330  
 C EXPLAN(J) = REAL\*4 ARRAY. ITS DIMENSION IS 20. THIS ARRAY IS LEV08340  
 C USED TO ALLOW EXPLANATORY COMMENTS IN THE INPUT FILES. LEV08350  
 C LEV08360  
 C G(J) = REAL\*4 ARRAY. ITS DIMENSION MUST BE >= MAX(2\*KMAX,N) LEV08370  
 C IT IS USED FOR HOLDING THE RANDOM VECTORS GENERATED, LEV08380  
 C HOLDING THE COMPUTED ERROR ESTIMATES AND THE COMPUTED LEV08390  
 C MINIMAL GAPS FOR THE GOOD T-EIGENVALUES. LEV08400  
 C LEV08410  
 C MP(J) = INTEGER\*4 ARRAY. ITS DIMENSION MUST BE AT LEAST KMAX, LEV08420  
 C THE MAXIMUM SIZE OF THE T-MATRICES ALLOWED. IT CONTAINS LEV08430  
 C THE T-MULTIPLICITIES OF THE COMPUTED EIGENVALUES. NOTE LEV08440  
 C THAT 'SPURIOUS' T-EIGENVALUES ARE DENOTED BY A LEV08450  
 C T-MULTIPLICITY OF 0. T-EIGENVALUES THAT THE SUBROUTINE LEV08460  
 C PRTEST HAS IDENTIFIED AS 'GOOD' BUT HIDDEN ARE IDENTIFIED LEV08470  
 C BY A T-MULTIPLICITY OF -10. LEV08480  
 C LEV08490  
 C NMEV(J) = INTEGER\*4 ARRAY. ITS DIMENSION MUST BE AT LEAST THE LEV08500  
 C NUMBER OF T-MATRICES ALLOWED. IT CONTAINS THE ORDERS LEV08510  
 C OF THE T-MATRICES TO BE CONSIDERED. LEV08520  
 C LEV08530  
 C LEV08540  
 C FOR CASE (3) ONLY: LEV08550  
 C GR(J),GC(J) = REAL\*8 ARRAYS. USED ONLY IN THE HERMITIAN CASE. LEV08560  
 C GR AND GC MUST EACH BE OF DIMENSION AT LEAST N. LEV08570  
 C BOTH ARE USED IN THE RANDOM VECTOR GENERATION. LEV08580  
 C GR IS ALSO USED TO STORE MINIMAL GAPS BETWEEN LEV08590  
 C 'GOOD' T-EIGENVALUES. LEV08600  
 C LEV08610  
 C FOR CASES (3) AND (4) FOR THE PERMUTATION: LEV08620  
 C LEV08630  
 C IPR(J), IPT(J) = INTEGER\*4 ARRAYS. EACH OF DIMENSION AT LEAST N. LEV08640  
 C USED TO STORE THE REORDERING OF THE GIVEN MATRIX LEV08650  
 C OR MATRICES. LEV08660  
 C LEV08670  
 C LEV08680  
 C OTHER ARRAYS LEV08690  
 C LEV08700  
 C THE USER MUST SPECIFY IN THE SUBROUTINE USPEC (A OR B) WHATEVER LEV08710  
 C ARRAYS ARE REQUIRED TO DEFINE THE MATRIX OR MATRICES BEING USED. LEV08720  
 C ALSO IN CASES (3) AND (4) ONLY, WHEN WORKING WITH INVERSES LEV08730  
 C OF SPARSE SYMMETRIC MATRICES, IN THE OPTIONAL, PREPROCESSING LEV08740  
 C PROGRAMS PERMUT, LFACT, LORDER, AND LTEST IT IS NECESSARY TO LEV08750  
 C SPECIFY ADDITIONAL ARRAYS JUST FOR THESE COMPUTATIONS. THE USER LEV08760

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C      IS REFERRED TO THOSE PROGRAMS FOR DETAILS.                                LEV08770
C                                                                                   LEV08780
C                                                                                   LEV08790
C-----SUBROUTINES INCLUDED-----LEV08800
C                                                                                   LEV08810
C                                                                                   LEV08820
C      LANCZS = COMPUTES THE ALPHA/BETA HISTORY. IN CASES (1) AND (2)             LEV08830
C      REAL SYMMETRIC AND HERMITIAN MATRICES, USES SUBROUTINES                     LEV08840
C      FINPRO, GENRAN AND CMATV. IN CASE (3), INVERSES OF                         LEV08850
C      REAL SYMMETRIC MATRICES, USES SUBROUTINES FINPRO,                         LEV08860
C      GENRAN AND BSOLV. IN CASE (4), GENERALIZED EIGENVALUE                     LEV08870
C      PROBLEM, USES SUBROUTINES FINPRO, GENRAN, AMATV AND                       LEV08880
C      LSOLV.                                                                     LEV08890
C                                                                                   LEV08900
C      BISEC = COMPUTES EIGENVALUES OF THE SPECIFIED T-MATRIX                     LEV08910
C      USING STURM SEQUENCING, ON SEQUENCE OF INTERVALS                         LEV08920
C      SPECIFIED BY THE USER. EACH SUBINTERVAL IS TREATED                       LEV08930
C      AS OPEN ON THE LEFT AND CLOSED ON THE RIGHT.                             LEV08940
C      EIGENVALUES ARE COMPUTED WITH SIMULTANEOUS DETERMINATION                 LEV08950
C      OF THE T-MULTIPLICITIES AND OF SPURIOUS T-EIGENVALUES.                   LEV08960
C                                                                                   LEV08970
C      INVERR = USES INVERSE ITERATION ON T-MATRICES TO COMPUTE ERROR            LEV08980
C      ESTIMATES ON COMPUTED GOOD T-EIGENVALUES. (USES GENRAN)                   LEV08990
C                                                                                   LEV09000
C      LUMP = 'COMBINES' EIGENVALUES OF T-MATRIX USING THE RELATIVE              LEV09010
C      TOLERANCE RELTOL.                                                         LEV09020
C                                                                                   LEV09030
C      ISOEV = CALCULATES GAPS BETWEEN DISTINCT EIGENVALUES OF T-MATRIX          LEV09040
C      AND THEN USES THESE GAPS TO LABEL THOSE 'GOOD'                           LEV09050
C      T-EIGENVALUES FOR WHICH ERROR ESTIMATES ARE NOT COMPUTED.                 LEV09060
C                                                                                   LEV09070
C      TNORM = COMPUTES THE SCALE TKMAX USED IN DETERMINING THE                  LEV09080
C      TOLERANCES FOR THE SPURIOUS, T-MULTIPLICITY AND PRTESTS.                 LEV09090
C      IT ALSO CHECKS FOR LOCAL ORTHOGONALITY OF THE LANCZOS                     LEV09100
C      VECTORS BY TESTING THE RELATIVE SIZE OF THE BETAS USING                   LEV09110
C      THE RELATIVE TOLERANCE BTOL.                                              LEV09120
C                                                                                   LEV09130
C      PRTEST = LOOKS FOR GOOD T-EIGENVALUES THAT HAVE BEEN MISLABELLED         LEV09140
C      BY THE SPURIOUS TEST BECAUSE THEY HAD 'TOO SMALL' A                      LEV09150
C      PROJECTION ON THE STARTING LANCZOS VECTOR.                               LEV09160
C      (LESS THAN SINGLE PRECISION)                                             LEV09170
C      TESTS INDICATE THAT SUCH EIGENVALUES ARE RARE.                           LEV09180
C      PRTEST SHOULD BE CALLED ONLY AFTER CONVERGENCE                           LEV09190
C      HAS BEEN ESTABLISHED.                                                    LEV09200
C                                                                                   LEV09210
C      INVERM = USED TO COMPUTE ERROR ESTIMATES FOR ANY T-EIGENVALUES            LEV09220
C      WHICH PRTEST INDICATES MAY HAVE BEEN MISLABELLED.                       LEV09230
C      SUCH T-EIGENVALUES ARE RELABELLED ONLY IF THEIR ERROR                     LEV09240
C      ESTIMATES ARE SUFFICIENTLY SMALL. PRIMARY USE OF                         LEV09250
C      INVERM IS IN THE CORRESPONDING EIGENVECTOR COMPUTATIONS.                 LEV09260
C                                                                                   LEV09270
C      CASES (3) AND (4) ONLY, FACTORED INVERSES:                               LEV09280
C                                                                                   LEV09290
C      FOR OPTIONAL, PRELIMINARY PROCESSING:                                    LEV09300
C      PERMUT (PROGRAM CALLS SPARSPAK PACKAGE) :                                LEV09310

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C      USES THE NONZERO STRUCTURE OF A GIVEN MATRIX A.                                LEV09320
C      CAN BE USED TO OBTAIN A REORDERING OF A THAT PRESERVES                       LEV09330
C      SPARSITY UNDER FACTORIZATION. PERMUT CALLS                                  LEV09340
C      THE SPARSPAK PROGRAMS, (A. GEORGE, J. LIU, E. NG,                            LEV09350
C      U. WATERLOO). PERMUT ALSO TAKES THE USER-SPECIFIED MATRIX,                  LEV09360
C      APPLIES THE SCALE SO AND THE SHIFT TO IT, AND THEN WRITES                   LEV09370
C      OUT THE CORRESPONDING SPARSE MATRIX DATA FILE FOR THE                      LEV09380
C      RESULTING MATRIX  $C = S0*A + SHIFT*I$ . SEE THE PERMUT FORTRAN                LEV09390
C      CODE FOR DETAILS.                                                            LEV09400
C                                                                                     LEV09410
C      LORDER (STAND-ALONE PROGRAM):                                               LEV09420
C      GIVEN A MATRIX C IN SPARSE FORMAT AND A PERMUTATION P,                      LEV09430
C      COMPUTES THE REORDERED MATRIX  $B = P*C*P'$  AND WRITES IT                     LEV09440
C      TO FILE 9 IN SPARSE FORMAT. SEE THE LORDER FORTRAN CODE                    LEV09450
C      FOR DETAILS.                                                                  LEV09460
C                                                                                     LEV09470
C      LFACT (STAND-ALONE PROGRAM) :                                              LEV09480
C      GIVEN A POSITIVE DEFINITE MATRIX B IN SPARSE FORMAT                        LEV09490
C      COMPUTES THE SPARSE CHOLESKY FACTOR L OF B AND WRITES IT                   LEV09500
C      TO FILE 7 IN SPARSE FORMAT. THUS,  $B = L*L'$ .                               LEV09510
C      SEE THE LFACT FORTRAN CODE FOR DETAILS.                                     LEV09520
C                                                                                     LEV09530
C      LTEST (CALLS 3 USER-SUPPLIED PROGRAMS CMATV, CMATS, AND BSOLV):            LEV09540
C      GIVEN THE FACTORIZATION OF A MATRIX B, LTEST COMPUTES                       LEV09550
C      THE SOLUTION OF THE EQUATION  $B*U = B*V1$  FOR A SPECIFIC RANDOMLY-          LEV09560
C      GENERATED V1, WITH AND WITHOUT ITERATIVE REFINEMENT, TO                   LEV09570
C      OBTAIN A ROUGH CHECK ON THE NUMERICAL CONDITION OF THE MATRIX B.           LEV09580
C      THIS PROGRAM USES 3 SUBROUTINES CMATV, CMATS, AND BLSOLV.                  LEV09590
C      SEE THE LTEST FORTRAN PROGRAM FOR DETAILS.                                  LEV09600
C                                                                                     LEV09610
C                                                                                     LEV09620
C-----OTHER PROGRAMS PROVIDED-----LEV09630
C                                                                                     LEV09640
C      LCOMPAC (STAND ALONE PROGRAM):                                             LEV09650
C          TRANSLATES A REAL SYMMETRIC MATRIX PROVIDED IN THE                     LEV09660
C          FORMAT I, J, A(I,J) INTO THE SPARSE MATRIX                            LEV09670
C          FORMAT USED IN THE SAMPLE USPEC, CMATV, BSOLV AND                      LEV09680
C          LSOLV SUBROUTINES PROVIDED. IT ASSUMES THAT THE                       LEV09690
C          MATRIX ENTRIES ARE GIVEN EITHER COLUMN BY COLUMN OR                   LEV09700
C          ROW BY ROW. THE DATA SET CREATED IS WRITTEN TO                       LEV09710
C          FILE 8.                                                                  LEV09720
C                                                                                     LEV09730
C                                                                                     LEV09740
C-----COMMENTS ON THE STORAGE REQUIRED FOR EIGENVALUE PROGRAMS-----LEV09750
C                                                                                     LEV09760
C                                                                                     LEV09770
C      CASE (1), REAL SYMMETRIC MATRICES:                                         LEV09780
C                                                                                     LEV09790
C      THE ARRAYS IN THE REAL SYMMETRIC EIGENVALUE PROGRAM REQUIRE                LEV09800
C      APPROXIMATELY THE EQUIVALENT OF ONE REAL*8 ARRAY OF DIMENSION             LEV09810
C                                                                                     LEV09820
C           $3.5*KMAX + 2*MAX(KMAX,N) + .5* MAX(2*KMAX,N)$                           LEV09830
C                                                                                     LEV09840
C      PLUS WHATEVER IS NEEDED TO GENERATE A*X FOR THE GIVEN MATRIX A.           LEV09850
C      THE ARRAYS ALPHA, BETA, VS AND MP CONSUME  $3.5*KMAX*8$  BYTES.              LEV09860

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C THE ARRAYS V1 AND V2 CONSUME  $2 * \text{MAXIMUM}(KMAX, N) * 8$  BYTES, WITH THE LEV09870  
 C QUALIFICATION STATED ABOVE WHERE V2 IS DEFINED. THE G-ARRAY LEV09880  
 C CONSUMES  $.5 * \text{MAX}(2 * KMAX, N) * 8$  BYTES. LEV09890  
 C LEV09900  
 C CASE (2), HERMITIAN MATRICES: LEV09910  
 C LEV09920  
 C THE ARRAYS IN THE HERMITIAN EIGENVALUE PROGRAMS REQUIRE LEV09930  
 C THE EQUIVALENT OF ONE REAL\*8 ARRAY OF DIMENSION LEV09940  
 C LEV09950  
 C  $3.5 * KMAX + 4 * \text{MAX}(KMAX/2, N) + .5 * \text{MAX}(2 * KMAX, N) + 2 * N$  LEV09960  
 C LEV09970  
 C PLUS WHATEVER IS NEEDED TO GENERATE  $A * X$  FOR THE GIVEN MATRIX A. LEV09980  
 C THE ARRAYS ALPHA, BETA, VS, AND MP CONSUME  $3.5 * KMAX * 8$  BYTES. LEV09990  
 C THE ARRAYS V1 AND V2 CONSUME  $4 * \text{MAXIMUM}(KMAX/2, N) * 8$  BYTES, WITH THE LEV10000  
 C QUALIFICATION STATED ABOVE WHERE V2 IS DEFINED. THE G-ARRAY LEV10010  
 C CONSUMES  $.5 * \text{MAX}(2 * KMAX, N) * 8$  BYTES. GR REQUIRES LEV10020  
 C AND GC REQUIRE  $2 * N * 8$  BYTES. LEV10030  
 C LEV10040  
 C LEV10050  
 C CASE (3), INVERSES OF REAL SYMMETRIC MATRICES: LEV10060  
 C LEV10070  
 C THE ARRAYS IN THE EIGENVALUE PROGRAMS DESIGNED FOR LEV10080  
 C CASE (3), INVERSES OF REAL SYMMETRIC MATRICES USING LEV10090  
 C REORDERING AND FACTORIZATION, REQUIRE LEV10100  
 C THE EQUIVALENT OF ONE REAL\*8 ARRAY OF DIMENSION LEV10110  
 C LEV10120  
 C  $3 * KMAX + 3 * \text{MAX}(KMAX, N) + .5 * \text{MAX}(2 * KMAX, N)$  LEV10130  
 C LEV10140  
 C PLUS WHATEVER IS NEEDED TO GENERATE  $B(\text{INVERSE}) * X$  FOR THE LEV10150  
 C SCALED, SHIFTED AND PERMUTED VERSION OF A WHICH WE DENOTE LEV10160  
 C BY B. THE ARRAYS ALPHA, BETA, MP, AND MP2 CONSUME  $3 * KMAX * 8$  LEV10170  
 C BYTES. THE ARRAYS V1, V2, AND VS CONSUME  $3 * \text{MAX}(KMAX, N) * 8$  BYTES, LEV10180  
 C WITH THE QUALIFICATION STATED ABOVE WHERE V2 IS DEFINED. LEV10190  
 C THE G ARRAY CONSUMES  $.5 * \text{MAX}(2 * KMAX, N) * 8$  BYTES. THESE NUMBERS LEV10200  
 C DO NOT INCLUDE THE STORAGE REQUIRED BY THE PREPROCESSING PROGRAMS LEV10210  
 C PERMUT, LORDER, LFACT, AND LTEST. LEV10220  
 C LEV10230  
 C LEV10240  
 C A SYMMETRIC, SPARSE MATRIX OF ORDER N WITH NZS NONZERO ELEMENTS LEV10250  
 C BELOW THE MAIN DIAGONAL WOULD REQUIRE THE EQUIVALENT OF ONE LEV10260  
 C REAL\*8 ARRAY OF DIMENSION  $1.5 * (NZS + N)$  IF THE POINTERS USED LEV10270  
 C ARE INTEGER\*4. LEV10280  
 C LEV10290  
 C SOME OF THE ARRAY STORAGE IS NOT ESSENTIAL AND COULD BE LEV10300  
 C ELIMINATED IF STORAGE IS A PROBLEM. LEV10310  
 C THE FOLLOWING COMMENTS APPLY DIRECTLY ONLY TO CASE (1), LEV10320  
 C THE PROGRAMS FOR REAL SYMMETRIC MATRICES, HOWEVER, SIMILAR LEV10330  
 C STATEMENTS COULD BE MADE ABOUT THE OTHER CASES. LEV10340  
 C LEV10350  
 C CASE (1), REAL SYMMETRIC PROGRAMS: LEV10360  
 C THE G ARRAY COULD BE REMOVED IF THE USER IS WILLING TO LEV10370  
 C LEV10380  
 C (1) REGENERATE THE RANDOM STARTING VECTOR IN INVERR LEV10390  
 C FOR EACH ERROR ESTIMATE LEV10400  
 C (2) WRITE OUT THE ERROR ESTIMATES AND VARIOUS GAPS AS LEV10410

C           THEY ARE GENERATED RATHER THAN STORING THEM IN G FOR    LEV10420  
 C           LATER PRINTOUT    LEV10430  
 C           (3) CHECK CONVERGENCE WITHIN INVERR                    LEV10440  
 C    LEV10450  
 C   CLEARLY THE INDEX VECTOR MP COULD BE AN INTEGER\*2 ARRAY AS COULD   LEV10460  
 C   THE POINTERS USED TO DEFINE THE USER'S MATRIX.                LEV10470  
 C    LEV10480  
 C   THE USER SHOULD NOTE THAT WITH AN EIGENVALUE SUBROUTINE THAT    LEV10490  
 C   USES BISECTION (LIKE BISEC) IF MORE THAN 25% OF THE            LEV10500  
 C   EIGENVALUES ARE TO BE COMPUTED, THEN IT MAY BE MORE            LEV10510  
 C   ECONOMICAL TO USE THE EISPACK SUBROUTINE IMTQL1.                LEV10520  
 C   (SEE MATRIX EIGENSYSTEM ROUTINES-EISPACK GUIDE (2ND EDITION)    LEV10530  
 C   B.T. SMITH ET AL, SPRINGER-VERLAG, NEW YORK, 1976, P213.).    LEV10540  
 C   HOWEVER, IF THE SUBROUTINE IMTQL1 IS TO BE USED IN PLACE        LEV10550  
 C   OF BISEC, THEN NONTRIVIAL CHANGES IN THE LANCZOS CODE MUST BE    LEV10560  
 C   MADE. FOR DETAILS OF ONE SUCH IMPLEMENTATION SEE                LEV10570  
 C   IBM RESEARCH REPORT 8298, COMPUTING                                LEV10580  
 C   EIGENVALUES OF LARGE SYMMETRIC MATRICES - AN IMPLEMENTATION OF A    LEV10590  
 C   LANCZOS ALGORITHM WITH NO REORTHOGONALIZATION. PART II. COMPUTER    LEV10600  
 C   PROGRAMS., DECEMBER 1980, WHICH CONTAINS A GENERAL                LEV10610  
 C   LANCZOS CODE WHICH INCLUDES AN IMTQL1 OPTION OR                 LEV10620  
 C   PREFERABLY CONTACT THE AUTHORS.                                    LEV10630  
 C    LEV10640  
 C   THE BISEC SUBROUTINE WHICH IS INCLUDED IS A MODIFIED FORM OF    LEV10650  
 C   THE BISECT SUBROUTINE IN EISPACK. BISEC ASSUMES THAT THE        LEV10660  
 C   VECTOR V2 IS LONG ENOUGH TO HOLD BOTH THE UPPER AND THE        LEV10670  
 C   LOWER BOUNDS ON THE BISECTION INTERVALS USED TO COMPUTE        LEV10680  
 C   THE EIGENVALUES OF THE T-MATRICES. THEREFORE, IF THE            LEV10690  
 C   LENGTH OF V2 IS ONLY KMAX, BISEC CAN COMPUTE ONLY AT MOST        LEV10700  
 C   KMAX/2 EIGENVALUES OF THE GIVEN T-MATRIX IN ANY GIVEN            LEV10710  
 C   SUBINTERVAL.    LEV10720  
 C    LEV10730  
 C   AS PROGRAMMED BISEC USES THE ARRAYS ALPHA,BETA,V1,V2,VS AND MP.    LEV10740  
 C   HOWEVER, V1 IS USED ONLY TO STORE BETA(J)\*\*2 SO THAT THEY DO NOT    LEV10750  
 C   HAVE TO BE REGENERATED ON EACH STURM. IF THE USER IS WILLING TO    LEV10760  
 C   COMPUTE THE BETA(J)\*\*2 AS NEEDED, THEN V1 COULD BE ELIMINATED    LEV10770  
 C   FROM BISEC. BISEC STORAGE THEN BECOMES A REAL\*8 ARRAY OF DIMENSION    LEV10780  
 C   4.25\*KMAX IF WE ALSO REDUCE MP TO INTEGER\*2. FURTHERMORE,        LEV10790  
 C   IF ONE KNEW THAT ONLY Q\*MEV EIGENVALUES OF T(1,MEV) WERE TO BE    LEV10800  
 C   COMPUTED AT EACH STAGE FOR SOME Q<.5 THEN FURTHER REDUCTIONS IN    LEV10810  
 C   STORAGE COULD BE MADE IN BISEC.                                    LEV10820  
 C    LEV10830  
 C   AS PROGRAMMED INVERR USES ALPHA, BETA,V1,V2,VS,G AND MP.        LEV10840  
 C   VS CONTAINS THE COMPUTED EIGENVALUES OF T(1,MEV). MP GIVES        LEV10850  
 C   THEIR T-MULTIPLICITIES AND FLAGS WHICH EIGENVALUES ARE TO HAVE    LEV10860  
 C   ERROR ESTIMATES COMPUTED. V2 IS USED FOR THE SOLUTION            LEV10870  
 C   VECTOR IN THE INVERSE ITERATION AND V1 FOR THE FACTORIZATION.    LEV10880  
 C   G CONTAINS THE RANDOMLY-GENERATED STARTING VECTOR FOR THE        LEV10890  
 C   INVERSE ITERATION. THE BASIC STORAGE FOR INVERR IS THEREFORE    LEV10900  
 C   A REAL\*8 ARRAY OF DIMENSION 4\*KMAX PLUS THE STORAGE NEEDED FOR    LEV10910  
 C   THE COMPUTED T-EIGENVALUES AND THEIR T-MULTIPLICITIES.            LEV10920  
 C    LEV10930  
 C   VS COULD BE USED TO STORE ONLY THOSE COMPUTED EIGENVALUES OF        LEV10940  
 C   T(1,MEV) THAT ARE OF INTEREST. IN THAT CASE THE DIMENSIONS OF VS    LEV10950  
 C   AND OF MP NEED NOT BE ANY LONGER THAN THE NUMBER OF SUCH        LEV10960

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C   EIGENVALUES. AS PROGRAMMED, ALL THE COMPUTED DISTINCT EIGENVALUES LEV10970
C   OF T(1,MEV) ARE STORED IN VS. THEREFORE TO TAKE ADVANTAGE OF LEV10980
C   SUCH A REDUCTION IN STORAGE THE USER WOULD HAVE TO MODIFY THAT LEV10990
C   PART OF THE PROGRAM AND ALSO COMMENT OUT THE CALL TO THE LEV11000
C   SUBROUTINE PRTEST. LEV11010
C   LEV11020
C   LEV11030
C-----LEV11040
C   LEV11050
C   COMMENTS FOR EIGENVECTOR COMPUTATIONS LEV11060
C   LEV11070
C-----LEV11080
C   LEV11090
C   LEV11100
C   THE EIGENVALUES WHOSE EIGENVECTORS ARE TO BE COMPUTED MUST LEV11110
C   HAVE BEEN COMPUTED USING THE CORRESPONDING LANCZOS EIGENVALUE LEV11120
C   PROGRAMS BECAUSE THE EIGENVECTOR PROGRAMS WILL USE THE SAME LEV11130
C   FAMILY OF LANCZOS TRIDIAGONAL MATRICES THAT WAS USED IN THE LEV11140
C   CORRESPONDING EIGENVALUE COMPUTATIONS. LEV11150
C   LEV11160
C   THESE PROGRAMS ASSUME THAT THE EIGENVALUES SUPPLIED TO IT LEV11170
C   HAVE BEEN COMPUTED ACCURATELY, AS MEASURED BY THE LEV11180
C   ERROR ESTIMATES COMPUTED IN THE CORRESPONDING LANCZOS LEV11190
C   EIGENVALUE COMPUTATIONS, ALTHOUGH THESE ESTIMATES ARE LEV11200
C   TYPICALLY CONSERVATIVE. IN CASES (1), (2) AND (4), THE LEV11210
C   EIGENVALUES OF INTEREST ARE STORED IN THE ARRAY GOODEV(J), LEV11220
C   J=1,NGOOD. IN CASE (3) THE PROGRAM WORKS WITH THE LEV11230
C   EIGENVALUES OF B(INVERSE) WHICH ARE STORED IN THE ARRAY LEV11240
C   GOODBI(J), J=1,NGOOD. THE CORRESPONDING EIGENVALUES LEV11250
C   OF A ARE STORED IN GOODA(J), J=1,NGOOD. LEV11260
C   LEV11270
C   FOR EACH GOODEV(J), THE SUBROUTINE STURMI COMPUTES THE LEV11280
C   SMALLEST SIZE LANCZOS TRIDIAGONAL MATRIX, T(1,M1(J)), FOR LEV11290
C   WHICH GOODEV(J) IS AN EIGENVALUE TO WITHIN A SPECIFIED LEV11300
C   TOLERANCE. IT ALSO ATTEMPTS TO COMPUTE THE SIZE, M2(J), LEV11310
C   BY WHICH THE GIVEN EIGENVALUE BECOMES A DOUBLE EIGENVALUE LEV11320
C   TO WITHIN THE GIVEN TOLERANCE. THESE VALUES ARE USED LEV11330
C   TO DETERMINE 1ST GUESSES AT SIZES FOR THE T-EIGENVECTORS LEV11340
C   THAT WILL BE USED IN THE RITZ VECTOR COMPUTATIONS. LEV11350
C   SUBROUTINE INVERM SUCCESSIVELY COMPUTES CORRESPONDING LEV11360
C   EIGENVECTORS OF ENLARGED T-MATRICES UNTIL A SUITABLE LEV11370
C   SIZE T-MATRIX IS DETERMINED FOR EACH J. UP TO 10 SUCH LEV11380
C   EIGENVECTOR COMPUTATIONS ARE ALLOWED FOR EACH EIGENVALUE. LEV11390
C   LEV11400
C   AFTER APPROPRIATE T-EIGENVECTORS HAVE BEEN COMPUTED, LEV11410
C   RITZ VECTOR CORRESPONDING TO THESE T-EIGENVECTORS ARE THEN LEV11420
C   COMPUTED AND TAKEN AS APPROXIMATE EIGENVECTORS OF A FOR THE LEV11430
C   GIVEN EIGENVALUES, GOODEV(J), J = 1, ..., NGOOD. LEV11440
C   LEV11450
C   THIS IMPLEMENTATION FIRST COMPUTES ALL OF THE RELEVANT LEV11460
C   EIGENVECTORS OF THE SYMMETRIC TRIDIAGONAL MATRICES LEV11470
C   IN THE VECTOR, TVEC. LEV11480
C   LEV11490
C   THEN, AS EACH OF THE LANCZOS VECTORS IS REGENERATED, ALL LEV11500
C   OF THE RITZ VECTORS CORRESPONDING TO THESE LEV11510

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C      T-EIGENVECTORS ARE UPDATED USING THE CURRENTLY-GENERATED          LEV11520
C      LANCZOS VECTOR.  LANCZOS VECTORS ARE GENERATED (NOTE             LEV11530
C      THAT THEY ARE NOT BEING KEPT), UNTIL ENOUGH HAVE                 LEV11540
C      BEEN GENERATED TO MAP THE LONGEST T-EIGENVECTOR INTO ITS        LEV11550
C      CORRESPONDING RITZ VECTOR.  THE ARRAY RITVEC CONTAINS THE        LEV11560
C      SUCCESSIVE RITZ VECTORS WHICH ARE THE APPROXIMATE                 LEV11570
C      EIGENVECTORS OF A.                                              LEV11580
C                                                                      LEV11590
C                                                                      LEV11600
C-----PARAMETER CONTROLS FOR EIGENVECTOR PROGRAMS-----LEV11610
C                                                                      LEV11620
C                                                                      LEV11630
C      IN CASES (3) AND (4) WHERE A SPARSE FACTORIZATION OF A          LEV11640
C      SPECIFIED MATRIX IS USED, THE USER SPECIFIES USING THE FLAG     LEV11650
C      JPERM WHETHER OR NOT THE FACTORIZATION SUPPLIED CORRESPONDS     LEV11660
C      TO THE ORIGINAL MATRIX OR TO A PERMUTATION OF THE ORIGINAL      LEV11670
C      MATRIX.                                                           LEV11680
C                                                                      LEV11690
C      JPERM = (0,1) MEANS                                              LEV11700
C          0  NO PERMUTATION                                             LEV11710
C          1  MATRIX HAS BEEN PERMUTED.  NOTE THAT IN                   LEV11720
C              CASE (4) THE PROGRAM WILL ASSUME THAT THE                 LEV11730
C              DATA SUPPLIED FOR THE A-MATRIX CORRESPONDS TO THE      LEV11740
C              CORRESPONDING PERMUTATION OF THE ORIGINAL A-MATRIX.     LEV11750
C              IN BOTH CASES THE LANCZS CODES WILL WORK WITH THE      LEV11760
C              PERMUTED MATRICES AND THE PERMUTATION WILL BE          LEV11770
C              UNDONE ONLY IN THE EIGENVECTOR PROGRAM AFTER            LEV11780
C              THE RITZ VECTORS FOR THE PERMUTED PROBLEM HAVE          LEV11790
C              BEEN COMPUTED.                                           LEV11800
C                                                                      LEV11810
C      OTHER PARAMETER CONTROLS ARE INTRODUCED TO ALLOW SEGMENTATION    LEV11820
C      OF THE EIGENVECTOR COMPUTATIONS AND TO ALLOW VARIOUS COMBINATIONS LEV11830
C      OF READ/Writes.                                                 LEV11840
C                                                                      LEV11850
C      THE FLAG MBOUND ALLOWS THE USER TO DETERMINE A FIRST GUESS ON THE LEV11860
C      STORAGE THAT WILL BE REQUIRED BY THE T-EIGENVECTORS FOR THE      LEV11870
C      EIGENVALUES WHOSE EIGENVECTORS ARE TO BE COMPUTED.             LEV11880
C      THIS CAN BE USED TO ESTIMATE THE REQUIRED SIZE OF THE TVEC ARRAY. LEV11890
C                                                                      LEV11900
C      MBOUND = (0,1) MEANS                                             LEV11910
C                                                                      LEV11920
C          (0) PROGRAM COMPUTES FIRST GUESSES AT THE SIZES              LEV11930
C              OF THE T-MATRICES REQUIRED BY EACH OF THE                 LEV11940
C              EIGENVALUES SUPPLIED AND THEN CONTINUES WITH           LEV11950
C              THE CORRESPONDING T-EIGENVECTOR COMPUTATIONS.          LEV11960
C                                                                      LEV11970
C          (1) PROGRAM COMPUTES FIRST GUESSES AT THE SIZES              LEV11980
C              OF THE T-MATRICES REQUIRED BY EACH OF THE                 LEV11990
C              EIGENVALUES SUPPLIED, STORES THESE IN FILE 10          LEV12000
C              AND THEN TERMINATES.  THE USER CAN USE THESE           LEV12010
C              SIZES TO ESTIMATE THE SIZE TVEC ARRAY NEEDED           LEV12020
C              FOR THE DESIRED T-EIGENVECTOR COMPUTATIONS.            LEV12030
C                                                                      LEV12040
C      THE FLAGS NTVCON, TVSTOP, LVCONT, AND ERCONT CONTROL THE STOPPING LEV12050
C      CRITERIA FOR INTERMEDIATE POINTS IN THE LANCZOS PROCEDURE.  THEY LEV12060

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C	TERMINATE THE PROCEDURE IF VARIOUS QUANTITIES COULD NOT BE	LEV12070
C	COMPUTED AS DESIRED.	LEV12080
C		LEV12090
C	NTVCON = (0,1) MEANS	LEV12100
C		LEV12110
C	(0) IF THE ESTIMATED STORAGE FOR THE T-EIGENVECTORS	LEV12120
C	EXCEEDS THE USER-SPECIFIED DIMENSION OF THE	LEV12130
C	TVEC ARRAY PROGRAM DOES NOT CONTINUE WITH THE	LEV12140
C	T-EIGENVECTOR COMPUTATIONS. TERMINATION OCCURS.	LEV12150
C		LEV12160
C	(1) CONTINUE WITH THE T-EIGENVECTOR COMPUTATIONS	LEV12170
C	EVEN IF THE ESTIMATED STORAGE FOR TVEC EXCEEDS	LEV12180
C	THE USER-SPECIFIED DIMENSION OF THE TVEC ARRAY.	LEV12190
C	IN THIS SITUATION THE PROGRAM COMPUTES AS MANY	LEV12200
C	T-EIGENVECTORS AS IT HAS ROOM FOR, IN THE SAME	LEV12210
C	ORDER IN WHICH THE EIGENVALUES ARE PROVIDED.	LEV12220
C		LEV12230
C	SVTVEC = (0,1) MEANS	LEV12240
C		LEV12250
C	(0) DO NOT STORE THE COMPUTED T-EIGENVECTORS ON	LEV12260
C	FILE 11 UNLESS ALSO HAVE THE FLAG TVSTOP = 1,	LEV12270
C	IN WHICH CASE THE T-EIGENVECTORS ARE ALWAYS	LEV12280
C	WRITTEN TO FILE 11.	LEV12290
C		LEV12300
C	(1) STORE THE COMPUTED T-EIGENVECTORS ON FILE 11.	LEV12310
C		LEV12320
C	TVSTOP = (0,1) MEANS	LEV12330
C		LEV12340
C	(0) ATTEMPT TO CONTINUE ON TO THE COMPUTATION	LEV12350
C	OF THE RITZVECTORS AFTER COMPLETING THE	LEV12360
C	COMPUTATION OF THE T-EIGENVECTORS.	LEV12370
C		LEV12380
C	(1) TERMINATE AFTER COMPUTING THE	LEV12390
C	T-EIGENVECTORS AND STORING THEM ON FILE 11.	LEV12400
C		LEV12410
C	LVCNT = (0,1) MEANS	LEV12420
C		LEV12430
C	(0) IF SOME OF THE T-EIGENVECTORS THAT WERE	LEV12440
C	REQUESTED WERE NOT COMPUTED, EXIT	LEV12450
C	FROM THE PROGRAM WITHOUT COMPUTING THE	LEV12460
C	CORRESPONDING RITZ VECTORS.	LEV12470
C		LEV12480
C	(1) CONTINUE ON TO THE RITZ VECTOR COMPUTATIONS	LEV12490
C	EVEN IF NOT ALL OF THE T-EIGENVECTORS	LEV12500
C	REQUESTED WERE COMPUTED.	LEV12510
C		LEV12520
C	ERCONT = (0,1) MEANS	LEV12530
C		LEV12540
C	(0) PROCEDURE WILL NOT COMPUTE A RITZ VECTOR FOR	LEV12550
C	ANY EIGENVALUE FOR WHICH NO T-EIGENVECTOR WHICH	LEV12560
C	SATISFIES THE ERROR ESTIMATE TEST (ERTOL) HAS	LEV12570
C	BEEN IDENTIFIED.	LEV12580
C		LEV12590
C	(1) A RITZ VECTOR WILL BE COMPUTED FOR EVERY	LEV12600
C	EIGENVALUE FOR WHICH A T-EIGENVECTOR HAS BEEN	LEV12610

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C          COMPUTED REGARDLESS OF WHETHER OR NOT THAT          LEV12620
C          T-EIGENVECTOR SATISFIED THE ERROR ESTIMATE TEST.    LEV12630
C                                                                LEV12640
C                                                                LEV12650
C-----INPUT/OUTPUT FILES FOR THE EIGENVECTOR COMPUTATIONS-----LEV12660
C                                                                LEV12670
C                                                                LEV12680
C  ANY INPUT DATA OTHER THAN THE T-MATRIX HISTORY FILE AND THE LEV12690
C  PREVIOUSLY COMPUTED EIGENVALUES AND CORRESPONDING ERROR      LEV12700
C  ESTIMATES SHOULD BE STORED ON FILE 5 IN FREE FORMAT.        LEV12710
C  SEE SAMPLE INPUT/OUTPUT FOR TYPICAL INPUT FILE.             LEV12720
C                                                                LEV12730
C  FILE 6 WAS USED AS THE INTERACTIVE TERMINAL OUTPUT FILE.    LEV12740
C  THIS FILE PROVIDES A RUNNING ACCOUNT OF THE PROGRESS OF THE LEV12750
C  COMPUTATIONS.  ADDITIONAL PRINTOUT IS GENERATED WHEN       LEV12760
C  THE FLAG IWRITE = 1.                                        LEV12770
C                                                                LEV12780
C                                                                LEV12790
C DESCRIPTION OF OTHER I/O FILES                                LEV12800
C                                                                LEV12810
C FILE (K)   CONTAINS:                                         LEV12820
C                                                                LEV12830
C   (2)     INPUT FILE:                                         LEV12840
C           PREVIOUSLY-GENERATED T-MATRICES (ALPHA/BETA ARRAYS) LEV12850
C           AND THE FINAL TWO LANCZOS VECTORS USED ON THAT      LEV12860
C           COMPUTATION.  THIS PROGRAM ALLOWS ENLARGEMENT      LEV12870
C           OF ANY T-MATRICES PROVIDED ON FILE 2.  NOTE THAT   LEV12880
C           IN CASE (4), THREE 'LANCZOS' VECTORS ARE ON FILE 2. LEV12890
C                                                                LEV12900
C   (3)     INPUT FILE:                                         LEV12910
C           THE GOOD EIGENVALUES OF THE T-MATRIX T(1,MEV)      LEV12920
C           FOR WHICH RITZ VECTORS ARE REQUESTED.              LEV12930
C           FILE 3 ALSO CONTAINS THE T-MULTIPLICITIES OF THESE LEV12940
C           EIGENVALUES AND THEIR COMPUTED GAPS IN THE         LEV12950
C           T-MATRICES AND IN THE USER-SUPPLIED MATRIX.  IN   LEV12960
C           CASE (3) FILE 3 CONTAINS THE EIGENVALUES OF THE    LEV12970
C           B-INVERSE MATRIX AND 3 SETS OF CORRESPONDING GAPS. LEV12980
C           THIS FILE IS CREATED IN THE LANCZOS EIGENVALUE     LEV12990
C           COMPUTATIONS.                                       LEV13000
C                                                                LEV13010
C   (4)     INPUT FILE:                                         LEV13020
C           ERROR ESTIMATES FOR THE ISOLATED GOOD T-EIGENVALUES LEV13030
C           ON FILE 3.  THIS FILE IS CREATED DURING THE LANCZOS LEV13040
C           EIGENVALUE COMPUTATIONS.                            LEV13050
C                                                                LEV13060
C   (7)     INPUT FILE:                                         LEV13070
C           IN CASE (3) ((4)),                                  LEV13080
C           CONTAINS SPARSE MATRIX REPRESENTATION OF FACTORIZATION LEV13090
C           OF MATRIX (B-MATRIX) USED BY LANCZS SUBROUTINE.    LEV13100
C                                                                LEV13110
C   (8)     INPUT FILE:                                         LEV13120
C           IN CASES (1),(2) AND (4), USPEC SUBROUTINE ASSUMES LEV13130
C           THAT USER-SUPPLIED A-MATRIX IS ON FILE 8.  IN CASE (3) LEV13140
C           A-MATRIX CAN BE STORED ON FILE 8, BUT IT IS NOT    LEV13150
C           USED BY THE LANCZOS PROGRAMS.                       LEV13160

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C                                                    LEV13170
C   (9)   OUTPUT FILE:                               LEV13180
C         ERROR ESTIMATES FOR THE COMPUTED RITZ VECTORS CONSIDERED LEV13190
C         AS EIGENVECTORS OF THE MATRIX USED BY THE LANCZS      LEV13200
C         SUBROUTINE. THESE ESTIMATES ARE OF THE FORM          LEV13210
C           AERROR = || A*RITVEC - EVAL*RITVEC ||              LEV13220
C         WHERE A DENOTES THE MATRIX USED BY LANCZS, EVAL DENOTES LEV13230
C         THE EIGENVALUE BEING CONSIDERED AND RITVEC DENOTES   LEV13240
C         THE COMPUTED RITZ VECTOR.                           LEV13250
C                                                    LEV13260
C   (10)  OUTPUT FILE:                               LEV13270
C         GUESSES AT APPROPRIATE SIZE T-MATRICES FOR THE      LEV13280
C         T-EIGENVECTORS FOR EACH SUPPLIED EIGENVALUE, GOODEV(J). LEV13290
C                                                    LEV13300
C   (11)  OUTPUT FILE:                               LEV13310
C         COMPUTED T-EIGENVECTORS CORRESPONDING TO EIGENVALUES LEV13320
C         IN THE GOODEV ARRAY. NOTE THAT IT IS POSSIBLE IN    LEV13330
C         CERTAIN SITUATIONS THAT FOR SOME EIGENVALUES IN THE  LEV13340
C         GOODEV ARRAY A T-EIGENVECTOR WILL NOT BE COMPUTED.  LEV13350
C                                                    LEV13360
C   (12)  OUTPUT FILE:                               LEV13370
C         CONTAINS COMPUTED RITZ VECTORS CORRESPONDING TO     LEV13380
C         THE T-EIGENVECTORS ON FILE 11. NOTE THAT IN         LEV13390
C         SOME SITUATIONS THAT FOR SOME EIGENVALUES IN       LEV13400
C         THE GOODEV ARRAY FOR WHICH T-EIGENVECTORS HAVE    LEV13410
C         BEEN COMPUTED NO RITZ VECTOR WILL HAVE BEEN        LEV13420
C         COMPUTED.                                           LEV13430
C                                                    LEV13440
C   (13)  OUTPUT FILE:                               LEV13450
C         ADDITIONAL INFORMATION ABOUT THE BOUNDS AND ERROR  LEV13460
C         ESTIMATES OBTAINED.                                 LEV13470
C                                                    LEV13480
C                                                    LEV13490
C-----SEEDS FOR EIGENVECTOR PROGRAMS-----LEV13500
C                                                    LEV13510
C   SEEDS FOR RANDOM NUMBER GENERATOR GENRAN                LEV13520
C     (1) SVSEED = INTEGER*4 SCALAR USED IN THE SUBROUTINE  LEV13530
C           GENRAN TO GENERATE THE STARTING VECTOR FORLEV13540
C           THE REGENERATION OF THE LANCZOS VECTORS.        LEV13550
C                                                    LEV13560
C     (2) RHSEED = INTEGER*4 SCALAR USED IN THE SUBROUTINE  LEV13570
C           GENRAN TO GENERATE A RANDOM VECTOR FOR          LEV13580
C           USE IN SUBROUTINE INVERM.                       LEV13590
C                                                    LEV13600
C   USER SHOULD NOTE THAT SVSEED MUST BE THE SAME SEED THAT LEV13610
C   WAS USED TO GENERATE THE T-MATRICES THAT WERE USED TO  LEV13620
C   COMPUTE THE EIGENVALUES WHOSE EIGENVECTORS ARE TO BE COMPUTED. LEV13630
C   SVSEED IS READ IN FROM FILE 3.                          LEV13640
C                                                    LEV13650
C                                                    LEV13660
C-----USER-SPECIFIED PARAMETERS FOR THE EIGENVECTOR PROGRAMS-----LEV13670
C                                                    LEV13680
C                                                    LEV13690
C   NGOOD  = NUMBER OF EIGENVALUES READ INTO THE GOODEV ARRAY LEV13700
C           READ FROM FILE 3.                                LEV13710

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C		LEV13720
C	N = SIZE OF THE USER-SUPPLIED MATRIX.	LEV13730
C		LEV13740
C	MEV = SIZE OF THE T-MATRIX THAT WAS USED TO COMPUTE	LEV13750
C	THE EIGENVALUES WHOSE EIGENVECTORS ARE REQUESTED.	LEV13760
C	MEV IS READ IN FROM FILE 3.	LEV13770
C		LEV13780
C	KMAX = SIZE OF THE T-MATRIX PROVIDED ON FILE 2.	LEV13790
C		LEV13800
C	MDIMTV = MAXIMUM CUMULATIVE SIZE OF THE TVEC ARRAY ALLOWED	LEV13810
C	FOR ALL OF THE T-EIGENVECTORS REQUIRED. MDIMTV	LEV13820
C	MUST NOT EXCEED THE USER-SPECIFIED DIMENSION OF	LEV13830
C	THE TVEC ARRAY. PROGRAM CAN BE RUN WITH THE FLAG	LEV13840
C	MBOUND = 1 TO DETERMINE AN EDUCATED GUESS ON AN	LEV13850
C	APPROPRIATE DIMENSION FOR THE TVEC ARRAY.	LEV13860
C		LEV13870
C	MDIMRV = MAXIMUM CUMULATIVE SIZE OF THE RITVEC ARRAY ALLOWED	LEV13880
C	FOR ALL OF THE RITZ VECTORS TO BE COMPUTED. MDIMRV	LEV13890
C	MUST NOT EXCEED THE USER-SPECIFIED DIMENSION OF	LEV13900
C	THE RITVEC ARRAY. MUST BE SELECTED SO THAT	LEV13910
C	THERE IS ENOUGH ROOM FOR A RITZ VECTOR FOR EVERY	LEV13920
C	GOODEV(J) READ INTO PROGRAM. ( $\geq$ NGOOD*N)	LEV13930
C		LEV13940
C		LEV13950
C	-----ARRAYS REQUIRED BY THE EIGENVECTOR PROGRAMS-----	LEV13960
C		LEV13970
C		LEV13980
C	ALL 4 CASES	LEV13990
C		LEV14000
C	ALPHA(J) = REAL*8 ARRAY. ITS DIMENSION MUST BE AT LEAST	LEV14010
C	KMAXN, THE LARGEST SIZE T-MATRIX CONSIDERED BY	LEV14020
C	THE PROGRAM. NOTE THAT KMAXN IS THE LARGER OF	LEV14030
C	THE SIZE OF THE ALPHA, BETA HISTORY PROVIDED	LEV14040
C	ON FILE 2 (IF ANY ) AND THE SIZE WHICH THE PROGRAM	LEV14050
C	SPECIFIES INTERNALLY, THIS LATTER IS ALWAYS	LEV14060
C	$< = 11*MEV / 8 + 12$ , WHERE MEV IS THE SIZE	LEV14070
C	T-MATRIX THAT WAS USED IN THE CORRESPONDING EIGENVALUE	LEV14080
C	COMPUTATIONS. ALPHA CONTAINS THE DIAGONAL ENTRIES	LEV14090
C	OF THE LANCZOS T-MATRICES. ALPHA IS NOT DESTROYED	LEV14100
C	IN THE COMPUTATIONS.	LEV14110
C		LEV14120
C	BETA(J) = REAL*8 ARRAY. ITS DIMENSION MUST BE AT LEAST 1	LEV14130
C	MORE THAN THAT OF ALPHA. DIMENSION COMMENTS ABOVE	LEV14140
C	ABOUT ALPHA APPLY ALSO TO THE BETA ARRAY. BETA	LEV14150
C	CONTAINS THE SUBDIAGONAL ENTRIES OF THE T-MATRICES.	LEV14160
C	BETA IS NOT DESTROYED IN THE COMPUTATIONS.	LEV14170
C		LEV14180
C	RITVEC(J) = REAL*8 ARRAY IN REAL SYMMETRIC AND INVERSE OF	LEV14190
C	REAL SYMMETRIC CASES. COMPLEX*16 IN CASE (2),	LEV14200
C	HERMITIAN MATRICES. IN EACH CASE ITS DIMENSION $\geq$	LEV14210
C	NGOOD*N WHERE N IS THE ORDER OF THE USER-SUPPLIED	LEV14220
C	MATRIX AND NGOOD IS THE NUMBER OF EIGENVALUES WHOSE	LEV14230
C	EIGENVECTORS ARE TO BE COMPUTED. IT CONTAINS THE	LEV14240
C	COMPUTED APPROXIMATE EIGENVECTORS OF A. THESE	LEV14250
C	COMPUTED RITZ VECTORS ARE STORED ON FILE 12.	LEV14260

C		LEV14270
C	TVEC(J) = REAL*8 ARRAY. ITS DIMENSION MUST BE AT LEAST	LEV14280
C	MTOL =  MA(1)  +  MA(2)  + ... +  MA(NGOOD)	LEV14290
C	WHERE NGOOD IS THE NUMBER OF EIGENVALUES BEING	LEV14300
C	CONSIDERED AND  MA(J)  IS THE SIZE OF THE	LEV14310
C	T-MATRIX BEING USED FOR THE RITZ VECTOR	LEV14320
C	COMPUTATION FOR GOODEV(J). THESE SIZES	LEV14330
C	ARE COMPUTED BY THE PROGRAM. AN ESTIMATE OF	LEV14340
C	MTOL CAN BE OBTAINED BY SETTING MBOUND = 1,	LEV14350
C	RUNNING THE PROGRAM, AND MULTIPLYING THE RESULTING	LEV14360
C	TOTAL OF THE T-SIZES SPECIFIED BY 5/4. THE ARRAY	LEV14370
C	TVEC CONTAINS THE COMPUTED T-EIGENVECTORS. IF THE	LEV14380
C	FLAG SVTVEC = 1 OR THE FLAG TVSTOP = 1, THEN	LEV14390
C	THESE VECTORS ARE SAVED ON FILE 11.	LEV14400
C		LEV14410
C	V1(J) = REAL*8 ARRAY IN REAL SYMMETRIC AND INVERSE OF	LEV14420
C	REAL SYMMETRIC CASES. COMPLEX*16 IN CASE (2),	LEV14430
C	HERMITIAN MATRICES. IN THE REAL CASES ITS	LEV14440
C	DIMENSION MUST BE THE MAXIMUM OF KMAX AND N.	LEV14450
C	IN THE HERMITIAN CASE ITS DIMENSION MUST BE	LEV14460
C	THE MAXIMUM OF KMAX/2 AND N WHERE KMAX IS THE	LEV14470
C	LARGEST SIZE T-MATRIX THAT IS TO BE CONSIDERED	LEV14480
C	IN THE T-EIGENVECTOR COMPUTATIONS. V1 IS USED	LEV14490
C	IN THE SUBROUTINE INVERM AND IN THE REGENERATION	LEV14500
C	OF THE LANCZOS VECTORS.	LEV14510
C		LEV14520
C	V2(J) = REAL*8 ARRAY IN THE REAL SYMMETRIC AND INVERSE	LEV14530
C	OF REAL SYMMETRIC CASES. COMPLEX*16 IN CASE (2),	LEV14540
C	HERMITIAN MATRICES. IN CASES (1),(3) AND (4), ITS	LEV14550
C	DIMENSION MUST BE > = MAX(KMAX,N); IN CASE (2)	LEV14560
C	> = MAX(KMAX/2,N). IT IS USED IN THE REGENERATION	LEV14570
C	OF THE LANCZOS VECTORS AND IN SUBROUTINE INVERM.	LEV14580
C		LEV14590
C	GOODEV(J), = REAL*8 ARRAYS EACH OF DIMENSION AT LEAST NGOOD.	LEV14600
C	EVNEW(J) CONTAIN THE EIGENVALUES FOR WHICH EIGENVECTORS	LEV14610
C	ARE REQUESTED. EIGENVALUES IN GOODEV ARE READ	LEV14620
C	IN FROM FILE 3. IN CASE (3) GOODEV IS REPLACED	LEV14630
C	BY GOODA AND GOODBI ARRAYS, SEE BELOW.	LEV14640
C		LEV14650
C	AMINGP(J), = REAL*4 ARRAYS OF DIMENSION AT LEAST NGOOD.	LEV14660
C	TMINGP(J) CONTAIN, RESPECTIVELY, THE MINIMAL GAPS FOR	LEV14670
C	CORRESPONDING EIGENVALUES IN GOODEV ARRAY IN	LEV14680
C	A-MATRIX AND IN T-MATRIX.	LEV14690
C		LEV14700
C	TERR(J), ERR(J), = REAL*4 ARRAYS (EXCEPT TLAST WHICH IS	LEV14710
C	ERRDGP(J), TLAST(J) REAL*8). EACH MUST BE OF DIMENSION	LEV14720
C	RNORM(J), TBETA(J) AT LEAST NGOOD. USED TO STORE QUANTITIES	LEV14730
C	GENERATED DURING THE COMPUTATIONS FOR	LEV14740
C	LATER PRINTOUT.	LEV14750
C		LEV14760
C	G(J) = REAL*4 ARRAY WHOSE DIMENSION MUST BE AT LEAST	LEV14770
C	MAX(KMAX,N). USED IN SUBROUTINE GENRAN TO HOLD	LEV14780
C	RANDOM NUMBERS NEEDED FOR THE LANCZOS VECTOR	LEV14790
C	REGENERATION AND FOR THE INVERSE ITERATION	LEV14800
C	COMPUTATIONS IN THE SUBROUTINE INVERM.	LEV14810

C		LEV14820
C	MP(J) = INTEGER*4 ARRAY WHOSE DIMENSION IS AT LEAST NGOOD.	LEV14830
C	INITIALLY CONTAINS THE MULTIPLICITY OF THE EIGENVALUE	LEV14840
C	GOODEV(J) AS AN EIGENVALUE OF THE T-MATRIX T(1,MEV).	LEV14850
C	USED TO FLAG EIGENVALUES FOR WHICH NO T-EIGENVECTOR	LEV14860
C	OR NO RITZ VECTOR IS TO BE COMPUTED.	LEV14870
C		LEV14880
C	MA(J) = INTEGER*4 ARRAYS EACH OF WHOSE DIMENSIONS	LEV14890
C	IS AT LEAST NGOOD. USED IN DETERMINING	LEV14900
C	AN APPROPRIATE T-MATRIX FOR EACH EIGENVALUE	LEV14910
C	IN GOODEV ARRAY.	LEV14920
C		LEV14930
C	MINT(J),MFIN(J) = INTEGER*4 ARRAYS WHOSE DIMENSIONS MUST BE AT	LEV14940
C	LEAST NGOOD. USED TO POINT TO THE BEGINNINGS	LEV14950
C	AND THE ENDS OF THE COMPUTED EIGENVECTOR	LEV14960
C	OF THE T-MATRIX, T(1, MA(J) ).	LEV14970
C		LEV14980
C	IDELTA(J) = INTEGER*4 ARRAY WHOSE DIMENSION MUST BE AT	LEV14990
C	LEAST NGOOD. CONTAINS INCREMENTS USED IN LOOPS	LEV15000
C	ON APPROPRIATE SIZE T-MATRIX FOR THE T-EIGENVECTOR	LEV15010
C	COMPUTATIONS.	LEV15020
C		LEV15030
C		LEV15040
C	CASE (2) ONLY, HERMITIAN MATRICES:	LEV15050
C		LEV15060
C	GR(J),GC(J) = REAL*8 ARRAYS USED ONLY IN CASE (2),	LEV15070
C	HERMITIAN MATRICES. EACH MUST BE AT	LEV15080
C	LEAST MAX(N,KMAX). USED TO HOLD	LEV15090
C	STARTING VECTORS FOR LANCZS	LEV15100
C	COMPUTATIONS AND FOR INVERM SUBROUTINES.	LEV15110
C		LEV15120
C	CASES (3) AND (4) ONLY, FACTORED INVERSES OF REAL SYMMETRIC	LEV15130
C	MATRICES AND GENERALIZED EIGENVALUE PROBLEMS:	LEV15140
C		LEV15150
C	VS(J) = REAL*8 ARRAY WHOSE DIMENSION MUST BE AT LEAST N.	LEV15160
C	USED IN REGENERATION OF THE LANCZOS VECTORS.	LEV15170
C		LEV15180
C	IPR(J), IPT(J) = INTEGER*4 ARRAYS. EACH MUST BE OF DIMENSION	LEV15190
C	AT LEAST N, THE ORDER OF A. USED TO STORE	LEV15200
C	THE REORDERING OF THE GIVEN MATRIX.	LEV15210
C		LEV15220
C	CASE (3) ONLY, INVERSES OF REAL SYMMETRIC MATRICES:	LEV15230
C		LEV15240
C	GOODA(J), GOODBI(J) = REAL*8 ARRAYS. EACH MUST BE OF DIMENSION	LEV15250
C	AT LEAST NGOOD, THE NUMBER OF EIGENVALUES	LEV15260
C	BEING CONSIDERED. GOODA CONTAINS THE	LEV15270
C	EIGENVALUES OF A AND GOODBI CONTAINS THE	LEV15280
C	EIGENVALUES OF B(INVERSE). THE PROGRAM	LEV15290
C	WORKS DIRECTLY WITH THE GOODBI ARRAY.	LEV15300
C		LEV15310
C		LEV15320
C	-----SUBROUTINES INCLUDED FOR THE EIGENVECTOR COMPUTATIONS-----	LEV15330
C		LEV15340
C		LEV15350
C	STURMI = FOR EACH GIVEN EIGENVALUE GOODEV(J) DETERMINES	LEV15360



## 2.3 LEVAL: Main Program, Eigenvalue Computations

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C-----LEVAL (EIGENVALUES OF REAL SYMMETRIC MATRICES)-----LEV00010
C  Authors:  Jane Cullum and Ralph A. Willoughby (Deceased)      LEV00020
C           Los Alamos National Laboratory                       LEV00030
C           Los Alamos, New Mexico 87544                       LEV00040
C                                                                 LEV00050
C           E-mail:  cullumj@lanl.gov                           LEV00060
C                                                                 LEV00070
C  These codes are copyrighted by the authors.  These codes     LEV00080
C  and modifications of them or portions of them are NOT to be  LEV00090
C  incorporated into any commercial codes or used for any other LEV00100
C  commercial purposes such as consulting for other companies,  LEV00110
C  without legal agreements with the authors of these Codes.    LEV00120
C  If these Codes or portions of them are used in other scientific or LEV00130
C  engineering research works the names of the authors of these codes LEV00140
C  and appropriate references to their written work are to be    LEV00150
C  incorporated in the derivative works.                          LEV00160
C                                                                 LEV00170
C  This header is not to be removed from these codes.           LEV00180
C                                                                 LEV00190
C           REFERENCE: Cullum and Willoughby, Chapters 1,2,3,4    LEV00191
C           Lanczos Algorithms for Large Symmetric Eigenvalue Computations LEV00192
C           VOL. 1 Theory. Republished as Volume 41 in SIAM CLASSICS in LEV00193
C           Applied Mathematics, 2002. SIAM Publications,         LEV00194
C           Philadelphia, PA. USA                                 LEV00195
C                                                                 LEV00196
C                                                                 LEV00200
C  CONTAINS MAIN PROGRAM FOR COMPUTING DISTINCT EIGENVALUES OF  LEV00210
C  A REAL SYMMETRIC MATRIX USING LANCZOS TRIDIAGONALIZATION     LEV00220
C  WITHOUT REORTHOGONALIZATION.                                  LEV00230
C                                                                 LEV00240
C  PFORT VERIFIER IDENTIFIED THE FOLLOWING NONPORTABLE          LEV00250
C  CONSTRUCTIONS                                                LEV00260
C                                                                 LEV00270
C  1.  DATA/MACHEP/ STATEMENT                                  LEV00280
C  2.  ALL READ(5,*) STATEMENTS (FREE FORMAT)                   LEV00290
C  3.  FORMAT(20A4) USED WITH EXPLANATORY HEADER EXPLAN.       LEV00300
C  4.  HEXADEcimal FORMAT (4Z20) USED IN ALPHA/BETA FILES 1 AND 2. LEV00310
C                                                                 LEV00320
C-----LEV00330
C                                                                 LEV00340
C  DOUBLE PRECISION  ALPHA(5000),BETA(5001)                     LEV00350
C  DOUBLE PRECISION  V1(5001),V2(5000),VS(5000)                 LEV00360
C  DOUBLE PRECISION  LB(20),UB(20)                               LEV00370
C  DOUBLE PRECISION  BTOL,GAPTOL,TTOL,MACHEP,EPSM,RELTOL        LEV00380
C  DOUBLE PRECISION  SCALE1,SCALE2,SCALE3,SCALE4,BISTOL,CONTOL,MULTOL LEV00390
C  DOUBLE PRECISION  ONE,ZERO,TEMP,TKMAX,BETAM,BKMIN,TO,T1      LEV00400
C  REAL  G(10000),EXPLAN(20)                                     LEV00410
C  INTEGER  MP(5000),NMEV(20)                                    LEV00420
C  INTEGER  SVSEED,RHSEED,SVSOLD                                 LEV00430
C  INTEGER  IABS                                                LEV00440
C  REAL  ABS                                                     LEV00450
C  DOUBLE PRECISION  DABS,DSQRT,DFLOAT                           LEV00460

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```

EXTERNAL CMATV                                LEV00470
C                                               LEV00480
C-----LEV00490
DATA MACHEP/Z3410000000000000/              LEV00500
EPSM = 2.0D0*MACHEP                          LEV00510
C-----LEV00520
C                                               LEV00530
C ARRAYS MUST BE DIMENSIONED AS FOLLOWS:     LEV00540
C DIMENSION OF V2 ASSUMES THAT NO MORE THAN  LEV00550
C OF THE T-MATRICES ARE BEING COMPUTED IN ANY LEV00560
C SUB-INTERVALS BEING CONSIDERED. V2 CONTAINS LEV00570
C BOUNDS FOR EACH T-EIGENVALUE BEING COMPUTED LEV00580
C GIVEN INTERVAL.                            LEV00590
C                                               LEV00600
C 1. ALPHA: >= KMAX, BETA: >= (KMAX+1)       LEV00610
C 2. V1: >= MAX(N,KMAX+1)                    LEV00620
C 3. V2: >= MAX(N,KMAX)                     LEV00630
C 4. VS: >= KMAX                             LEV00640
C 5. G: >= MAX(N,2*KMAX)                    LEV00650
C 6. MP: >= KMAX                             LEV00660
C 7. LB,UB: >= NUMBER OF SUBINTERVALS SUPPLIED LEV00670
C TO BISEC.                                  LEV00680
C 8. NMEV: >= NUMBER OF T-MATRICES ALLOWED.  LEV00690
C 9. EXPLAN: DIMENSION IS 20.                LEV00700
C                                               LEV00710
C IMPORTANT TOLERANCES OR SCALES THAT ARE USED LEV00720
C THROUGHOUT THIS PROGRAM ARE THE FOLLOWING:  LEV00730
C SCALED MACHINE EPSILON: TTOL = TKMAX*EPSM WHERE LEV00740
C EPSM = 2*MACHINE EPSILON AND              LEV00750
C TKMAX = MAX(|ALPHA(J)|,BETA(J), J = 1,MEV) LEV00760
C BISEC CONVERGENCE TOLERANCE: BISTOL = DSQRT(1000+MEV)*TTOL LEV00770
C BISEC T-MULTIPLICITY TOLERANCE: MULTOL = (1000+MEV)*TTOL LEV00780
C LANCZOS CONVERGENCE TOLERANCE: CONTOL = BETA(MEV+1)*1.D-10 LEV00790
C-----LEV00800
C OUTPUT HEADER                               LEV00810
WRITE(6,10)                                   LEV00820
10 FORMAT(/' LANCZOS PROCEDURE FOR REAL SYMMETRIC MATRICES'/) LEV00830
C                                               LEV00840
C SET PROGRAM PARAMETERS                       LEV00850
C SCALEK ARE USED IN TOLERANCES NEEDED IN SUBROUTINES LUMP, LEV00860
C ISOEV AND PRTEST. USER MUST NOT MODIFY THESE SCALES. LEV00870
SCALE1 = 5.0D2                                LEV00880
SCALE2 = 5.0D0                                LEV00890
SCALE3 = 5.0D0                                LEV00900
SCALE4 = 1.0D4                                LEV00910
ONE = 1.0D0                                   LEV00920
ZERO = 0.0D0                                  LEV00930
BTOL = 1.0D-8                                 LEV00940
C BTOL = EPSM                                 LEV00950
GAPTOL = 1.0D-8                               LEV00960
ICONV = 0                                     LEV00970
MOLD = 0                                     LEV00980
MOLD1 = 1                                     LEV00990
ICT = 0                                       LEV01000
MMB = 0                                       LEV01010

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      IPROJ = 0
      LEV01020
C-----LEV01030
C   READ USER-SPECIFIED PARAMETERS FROM INPUT FILE 5 (FREE FORMAT)
      LEV01040
C
      LEV01050
C   READ USER-PROVIDED HEADER FOR RUN
      LEV01060
      READ(5,20) EXPLAN
      LEV01070
      WRITE(6,20) EXPLAN
      LEV01080
      READ(5,20) EXPLAN
      LEV01090
      WRITE(6,20) EXPLAN
      LEV01100
      20 FORMAT(20A4)
      LEV01110
C
      LEV01120
C   READ ORDER OF MATRICES (N) , MAXIMUM ORDER OF T-MATRIX (KMAX),
      LEV01130
C   NUMBER OF T-MATRICES ALLOWED (NMEVS), AND MATRIX IDENTIFICATION
      LEV01140
C   NUMBERS (MATNO)
      LEV01150
      READ(5,20) EXPLAN
      LEV01160
      READ(5,*) N,KMAX,NMEVS,MATNO
      LEV01170
C
      LEV01180
C   READ SEEDS FOR LANCZS AND INVERR SUBROUTINES (SVSEED AND RHSEED)
      LEV01190
C   READ MAXIMUM NUMBER OF ITERATIONS ALLOWED FOR EACH INVERSE
      LEV01200
C   ITERATION (MXINIT) AND MAXIMUM NUMBER OF STURM SEQUENCES
      LEV01210
C   ALLOWED (MXSTUR)
      LEV01220
      READ(5,20) EXPLAN
      LEV01230
      READ(5,*) SVSEED,RHSEED,MXINIT,MXSTUR
      LEV01240
C
      LEV01250
C   ISTART = (0,1):  ISTART = 0 MEANS ALPHA/BETA FILE IS NOT
      LEV01260
C   AVAILABLE.  ISTART = 1 MEANS ALPHA/BETA FILE IS AVAILABLE ON
      LEV01270
C   FILE 2.
      LEV01280
C   ISTOP = (0,1):  ISTOP = 0 MEANS PROCEDURE GENERATES ALPHA/BETA
      LEV01290
C   FILE AND THEN TERMINATES.  ISTOP = 1 MEANS PROCEDURE GENERATES
      LEV01300
C   ALPHAS/BETAS IF NEEDED AND THEN COMPUTES EIGENVALUES AND ERROR
      LEV01310
C   ESTIMATES AND THEN TERMINATES.
      LEV01320
      READ(5,20) EXPLAN
      LEV01330
      READ(5,*) ISTART,ISTOP
      LEV01340
C
      LEV01350
C   IHIS = (0,1):  IHIS = 0 MEANS ALPHA/BETA FILE IS NOT WRITTEN
      LEV01360
C   TO FILE 1.  IHIS = 1 MEANS ALPHA/BETA FILE IS WRITTEN TO FILE 1.
      LEV01370
C   IDIST = (0,1):  IDIST = 0 MEANS DISTINCT T-EIGENVALUES
      LEV01380
C   ARE NOT WRITTEN TO FILE 11.  IDIST = 1 MEANS DISTINCT
      LEV01390
C   T-EIGENVALUES ARE WRITTEN TO FILE 11.
      LEV01400
C   IWRITE = (0,1):  IWRITE = 0 MEANS NO INTERMEDIATE OUTPUT
      LEV01410
C   FROM THE COMPUTATIONS IS WRITTEN TO FILE 6.  IWRITE = 1 MEANS
      LEV01420
C   T-EIGENVALUES AND ERROR ESTIMATES ARE WRITTEN TO FILE 6
      LEV01430
C   AS THEY ARE COMPUTED.
      LEV01440
      READ(5,20) EXPLAN
      LEV01450
      READ(5,*) IHIS,IDIST,IWRITE
      LEV01460
C
      LEV01470
C   READ IN THE RELATIVE TOLERANCE (RELTOL) FOR USE IN THE
      LEV01480
C   SPURIOUS, T-MULTIPLICITY, AND PRTESTS.
      LEV01490
      READ(5,20) EXPLAN
      LEV01500
      READ(5,*) RELTOL
      LEV01510
C
      LEV01520
C   READ IN THE SIZES OF THE T-MATRICES TO BE CONSIDERED.
      LEV01530
      READ(5,20) EXPLAN
      LEV01540
      READ(5,*) (NMEV(J), J=1,NMEVS)
      LEV01550
C
      LEV01560

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      WRITE(1,130) (V2(I), I=1,N)
C
      IF (ISTOP.EQ.0) GO TO 540
C
160 CONTINUE
      BKMIN = BTOL
C
      WRITE(6,170)
170 FORMAT(/' T-MATRICES (ALPHA AND BETA) ARE NOW AVAILABLE'/)
C
C-----LEVO2770
C  SUBROUTINE TNORM CHECKS MIN(BETA)/(ESTIMATED NORM(A)) > BTOL .
C  IF THIS IS VIOLATED IB IS SET EQUAL TO THE NEGATIVE OF THE INDEX
C  OF THE MINIMAL BETA. IF(IB < 0) THEN SUBROUTINE TNORM IS
C  CALLED FOR EACH VALUE OF MEV TO DETERMINE WHETHER OR NOT THERE
C  IS A BETA IN THE T-MATRIX SPECIFIED THAT VIOLATES THIS TEST.
C  IF THERE IS SUCH A BETA THE PROGRAM TERMINATES FOR THE USER
C  TO DECIDE WHAT TO DO. THIS TEST CAN BE OVER-RIDDEN BY
C  SIMPLY MAKING BTOL SMALLER, BUT THEN THERE IS THE POSSIBILITY
C  THAT LOSSES IN THE LOCAL ORTHOGONALITY MAY HURT THE COMPUTATIONS.
C  BTOL = 1.D-8 IS HOWEVER A CONSERVATIVE CHOICE FOR BTOL.
C
C  TNORM ALSO COMPUTES TKMAX = MAX(|ALPHA(K)|,BETA(K), K=1,KMAX).
C  TKMAX IS USED TO SCALE THE TOLERANCES USED IN THE
C  T-MULTIPLICITY AND SPURIOUS TESTS IN BISEC. TKMAX IS ALSO USED IN
C  THE PROJECTION TEST FOR HIDDEN EIGENVALUES THAT HAD 'TOO SMALL'
C  A PROJECTION ON THE STARTING VECTOR.
C
      CALL TNORM(ALPHA,BETA,BKMIN,TKMAX,KMAX,IB)
C
C-----LEVO2970
C
      TTOL = EPSM*TKMAX
C
      LOOP ON THE SIZE OF THE T-MATRIX
C
180 CONTINUE
      MMB = MMB + 1
      MEV = NMEV(MMB)
C  IS MEV TOO LARGE ?
      IF(MEV.LE.KMAX) GO TO 200
      WRITE(6,190) MMB, MEV, KMAX
190 FORMAT(/' TERMINATE PRIOR TO CONSIDERING THE',I6,'TH T-MATRIX'/
1' BECAUSE THE SIZE REQUESTED',I6,' IS GREATER THAN THE MAXIMUM SIZ
1E ALLOWED',I6/)
      GO TO 540
C
200 MP1 = MEV + 1
      BETAM = BETA(MP1)
C
      IF (IB.GE.0) GO TO 210
C
      TO = BTOL
C
C-----LEVO3210

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      LOOP = NDIS                                LEV03770
      CALL LUMP(VS,RELTOL,MULTOL,SCALE2,MP,LOOP)  LEV03780
C                                              LEV03790
C-----LEV03800
C                                              LEV03810
      IF(NDIS.EQ.LOOP) GO TO 230                 LEV03820
C                                              LEV03830
      WRITE(6,220) NDIS, MEV, LOOP              LEV03840
220 FORMAT(/I6,' DISTINCT T-EIGENVALUES WERE COMPUTED IN BISEC AT MEV LEV03850
      1',I6/ 2X,' LUMP SUBROUTINE REDUCES NUMBER OF DISTINCT EIGENVALUES LEV03860
      10',I6)                                    LEV03870
C                                              LEV03880
230 CONTINUE                                    LEV03890
      NDIS = LOOP                                LEV03900
      BETA(MP1) = BETAM                          LEV03910
C                                              LEV03920
C-----LEV03930
C      THE SUBROUTINE ISOEV LABELS THOSE SIMPLE EIGENVALUES OF T(1,MEV) LEV03940
C      WITH VERY SMALL GAPS BETWEEN NEIGHBORING EIGENVALUES OF T(1,MEV) LEV03950
C      TO AVOID COMPUTING ERROR ESTIMATES FOR ANY SIMPLE GOOD           LEV03960
C      T-EIGENVALUE THAT IS TOO CLOSE TO A SPURIOUS EIGENVALUE.        LEV03970
C      ON RETURN FROM ISOEV, G CONTAINS CODED MINIMAL GAPS              LEV03980
C      BETWEEN THE DISTINCT EIGENVALUES OF T(1,MEV). (G IS REAL).      LEV03990
C      G(I) < 0 MEANS MINGAP IS DUE TO LEFT GAP G(I) > 0 MEANS DUE TO   LEV04000
C      RIGHT GAP. MP(I) = -1 MEANS THAT THE GOOD T-EIGENVALUE IS SIMPLE LEV04010
C      AND HAS A VERY SMALL MINGAP IN T(1,MEV) DUE TO A SPURIOUS       LEV04020
C      EIGENVALUE. NG = NUMBER OF GOOD T-EIGENVALUES.                  LEV04030
C      NISO = NUMBER OF ISOLATED GOOD T-EIGENVALUES.                    LEV04040
C                                              LEV04050
      CALL ISOEV(VS,GAPTOL,MULTOL,SCALE1,G,MP,NDIS,NG,NISO)             LEV04060
C                                              LEV04070
C-----LEV04080
C                                              LEV04090
      WRITE(6,240)NG,NISO,NDIS                    LEV04100
240 FORMAT(/I6,' GOOD T-EIGENVALUES HAVE BEEN COMPUTED'/           LEV04110
      1 I6,' OF THESE ARE T-ISOLATED'/           LEV04120
      2 I6,' = NUMBER OF DISTINCT T-EIGENVALUES COMPUTED'/)         LEV04130
C                                              LEV04140
C      DO WE WRITE DISTINCT EIGENVALUES OF T-MATRIX TO FILE 11?        LEV04150
      IF (IDIST.EQ.0) GO TO 280                    LEV04160
C                                              LEV04170
      WRITE(11,250) NDIS,NISO,MEV,N,SVSEED,MATNO  LEV04180
250 FORMAT(/4I6,I12,I8,' = NDIS,NISO,MEV,N,SVSEED,MATNO'/)        LEV04190
C                                              LEV04200
      WRITE(11,260) (MP(I),VS(I),G(I), I=1,NDIS) LEV04210
260 FORMAT(2(I3,E25.16,E12.3))                                       LEV04220
C                                              LEV04230
      WRITE(11,270) NDIS, (MP(I), I=1,NDIS)      LEV04240
270 FORMAT(/I6,' = NDIS, T-MULTIPLICITIES (0 MEANS SPURIOUS)'/      LEV04250
      (20I4))
C                                              LEV04260
280 CONTINUE                                    LEV04270
C                                              LEV04280
      IF (NISO.NE.0) GO TO 310                    LEV04290
C                                              LEV04300
      WRITE(4,290) MEV                                LEV04310

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290 FORMAT(/' AT MEV = ',I6,' THERE ARE NO ISOLATED T-EIGENVALUES'/ LEV04320
1' SO NO ERROR ESTIMATES WERE COMPUTED/') LEV04330
C LEV04340
WRITE(6,300) LEV04350
300 FORMAT(/' ALL COMPUTED GOOD T-EIGENVALUES ARE MULTIPLE'/ LEV04360
1' THEREFORE ALL SUCH EIGENVALUES ARE ASSUMED TO HAVE CONVERGED') LEV04370
C LEV04380
ICONV = 1 LEV04390
GO TO 350 LEV04400
C LEV04410
310 CONTINUE LEV04420
C LEV04430
C-----LEV04440
C SUBROUTINE INVERR COMPUTES ERROR ESTIMATES FOR ISOLATED GOOD LEV04450
C T-EIGENVALUES USING INVERSE ITERATION ON T(1,MEV). ON RETURN LEV04460
C G(J) = MINIMUM GAP IN T(1,MEV) FOR EACH VS(J), J=1,NDIS LEV04470
C G(MEV+I) = BETAM*|U(MEV)| = ERROR ESTIMATE FOR ISOLATED GOOD LEV04480
C T-EIGENVALUES, WHERE I = 1, NISO AND BETAM = BETA(MEV+1) LEV04490
C U(MEV) IS MEVTH COMPONENT OF THE UNIT EIGENVECTOR OF T LEV04500
C CORRESPONDING TO THE ITH ISOLATED GOOD T-EIGENVALUE. LEV04510
C A NEGATIVE ERROR ESTIMATE MEANS THAT FOR THAT PARTICULAR LEV04520
C EIGENVALUE THE INVERSE ITERATION DID NOT CONVERGE IN <= MXINIT LEV04530
C STEPS AND THAT THE CORRESPONDING ERROR ESTIMATE IS QUESTIONABLE. LEV04540
C LEV04550
C V2 CONTAINS THE ISOLATED GOOD T-EIGENVALUES LEV04560
C V1 CONTAINS THE MINGAPS TO THE NEAREST DISTINCT EIGENVALUE LEV04570
C OF T(1,MEV) FOR EACH ISOLATED GOOD T-EIGENVALUE IN V2. LEV04580
C VS CONTAINS THE NDIS DISTINCT EIGENVALUES OF T(1,MEV) LEV04590
C MP CONTAINS THE CORRESPONDING CODED T-MULTIPLICITIES LEV04600
C LEV04610
IT = MXINIT LEV04620
CALL INVERR(ALPHA,BETA,V1,V2,VS,EPSM,G,MP,MEV,MMB,NDIS,NISO,N, LEV04630
1 RHSEED,IT,IWRITE) LEV04640
C LEV04650
C-----LEV04660
C LEV04670
C SIMPLE CHECK FOR CONVERGENCE. CHECKS TO SEE IF ALL OF THE ERROR LEV04680
C ESTIMATES ARE SMALLER THAN CONTOL = BETAM*1.D-10. LEV04690
C IF THIS TEST IS SATISFIED, THEN CONVERGENCE FLAG, ICONV IS SET LEV04700
C TO 1. TYPICALLY ERROR ESTIMATES ARE VERY CONSERVATIVE. LEV04710
C LEV04720
WRITE(6,320) CONTOL LEV04730
320 FORMAT(/' CONVERGENCE IS TESTED USING THE CONVERGENCE TOLERANCE', LEV04740
1E13.4/) LEV04750
C LEV04760
II = MEV +1 LEV04770
IF = MEV+NISO LEV04780
DO 330 I = II,IF LEV04790
IF (ABS(G(I)).GT.CONTOL) GO TO 350 LEV04800
330 CONTINUE LEV04810
ICONV = 1 LEV04820
MMB = NMEVS LEV04830
C LEV04840
WRITE(6,340) CONTOL LEV04850
340 FORMAT(' ALL COMPUTED ERROR ESTIMATES WERE LESS THAN',E15.4/ LEV04860

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      1 ' THEREFORE PROCEDURE TERMINATES'//)                                LEV04870
C                                                                                   LEV04880
350 CONTINUE                                                                    LEV04890
C                                                                                   LEV04900
C   IF CONVERGENCE IS INDICATED, THAT IS ICONV = 1 ,THEN                       LEV04910
C   THE SUBROUTINE PRTEST IS CALLED TO CHECK FOR ANY CONVERGED                   LEV04920
C   T-EIGENVALUES THAT HAVE BEEN MISLABELLED AS SPURIOUS BECAUSE                 LEV04930
C   THE PROJECTION OF THEIR EIGENVECTOR(S) ON THE STARTING                       LEV04940
C   VECTOR WERE TOO SMALL.                                                       LEV04950
C   NUMERICAL TESTS INDICATE THAT SUCH EIGENVALUES ARE RARE.                   LEV04960
C   IF FOR SOME REASON MANY OF THESE HIDDEN EIGENVALUES APPEAR                 LEV04970
C   ON SOME RUN, YOU CAN BE CERTAIN THAT SOMETHING IS FOULED UP.               LEV04980
C                                                                                   LEV04990
      IF (ICONV.EQ.0) GO TO 480                                                  LEV05000
C                                                                                   LEV05010
C-----LEV05020
C                                                                                   LEV05030
      CALL PRTEST (ALPHA,BETA,VS,TKMAX,EPSM,RELTOL,SCALE3,SCALE4,                LEV05040
1 MP,NDIS,MEV,IPROJ)                                                            LEV05050
C                                                                                   LEV05060
C-----LEV05070
C                                                                                   LEV05080
      IF(IPROJ.EQ.0) GO TO 470                                                  LEV05090
C                                                                                   LEV05100
      IF(IDIST.EQ.1) WRITE(11,360) IPROJ                                        LEV05110
360 FORMAT(' SUBROUTINE PRTEST WANTS TO RELABEL',I6,' SPURIOUS T-EIGENLEV05120
1VALUES'/' WE ACCEPT RELABELLING ONLY IF LAST COMPONENT OF T-EIGENVLEV05130
1ECTOR IS L.T. 1.D-10'//)                                                    LEV05140
C                                                                                   LEV05150
      IIX = RHSEED                                                            LEV05160
C                                                                                   LEV05170
C-----LEV05180
C                                                                                   LEV05190
      CALL GENRAN(IIX,G,MEV)                                                  LEV05200
C                                                                                   LEV05210
C-----LEV05220
C                                                                                   LEV05230
      ITEN = -10                                                            LEV05240
      NISOM = NISO + MEV                                                    LEV05250
      IWRITO = IWRITE                                                       LEV05260
      IWRITE = 0                                                            LEV05270
C                                                                                   LEV05280
      DO 390 J = 1,NDIS                                                       LEV05290
      IF(MP(J).NE.ITEN) GO TO 390                                           LEV05300
      TO = VS(J)                                                            LEV05310
C                                                                                   LEV05320
C-----LEV05330
C                                                                                   LEV05340
      IT = MXINIT                                                            LEV05350
      CALL INVERM(ALPHA,BETA,V1,V2,TO,TEMP,T1,EPSM,G,MEV,IT,IWRITE)          LEV05360
C                                                                                   LEV05370
C-----LEV05380
C                                                                                   LEV05390
      IF(TEMP.LE.1.D-10) GO TO 380                                           LEV05400
C   ERROR ESTIMATE WAS NOT SMALL REJECT RELABELLING OF THIS EIGENVALUELEV05410

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C   WRITE THE GOOD T-EIGENVALUES TO FILE 3.  FIRST TRANSFER THEM      LEV05970
C   TO V2 AND THEIR T-MULTIPLICITIES TO THE CORRESPONDING POSITIONS  LEV05980
C   IN MP AND COMPUTE THE A-MINGAPS, THE MINIMAL GAPS BETWEEN THE   LEV05990
C   GOOD T-EIGENVALUES.  THESE GAPS WILL BE PUT IN THE ARRAY G.     LEV06000
C   SINCE G CURRENTLY CONTAINS THE MINIMAL GAPS BETWEEN THE DISTINCT LEV06010
C   EIGENVALUES OF THE T-MATRIX, THESE GAPS WILL FIRST BE          LEV06020
C   TRANSFERRED TO V1.  NOTE THAT V1<0 MEANS THAT THAT MINIMAL GAP  LEV06030
C   IN THE T-MATRIX IS DUE TO A SPURIOUS T-EIGENVALUE.           LEV06040
C   ALL THIS INFORMATION IS PRINTED TO FILE 3                     LEV06050
C                                                                    LEV06060
480 CONTINUE                                                       LEV06070
C                                                                    LEV06080
   NG = 0                                                            LEV06090
   DO 490 I = 1,NDIS                                                LEV06100
   IF (MP(I).EQ.0) GO TO 490                                        LEV06110
   NG = NG+1                                                        LEV06120
   MP(NG) = MP(I)                                                  LEV06130
   V2(NG) = VS(I)                                                  LEV06140
   TEMP = G(I)                                                      LEV06150
   TEMP = DABS(TEMP)                                                LEV06160
   J = I+1                                                           LEV06170
   IF (G(I).LT.ZERO) J = I-1                                       LEV06180
   IF (MP(J).EQ.0) TEMP = -TEMP                                     LEV06190
   V1(NG) = TEMP                                                    LEV06200
490 CONTINUE                                                       LEV06210
C                                                                    LEV06220
   WRITE(6,500)MEV                                                 LEV06230
500 FORMAT(// ' T-EIGENVALUE CALCULATION AT MEV = ',I6,' IS COMPLETE LEV06240
1')                                                                 LEV06250
C                                                                    LEV06260
C   NG = NUMBER OF COMPUTED DISTINCT GOOD T-EIGENVALUES.  NEXT     LEV06270
C   GENERATE GAPS BETWEEN GOOD T-EIGENVALUES (AMINGAPS) AND PUT THEM LEV06280
C   IN G.  G(J) < 0 MEANS THE AMINGAP IS DUE TO THE LEFT-HAND GAP. LEV06290
C                                                                    LEV06300
   NGM1 = NG - 1                                                    LEV06310
   G(NG) = V2(NGM1)-V2(NG)                                         LEV06320
   G(1) = V2(2)-V2(1)                                              LEV06330
C                                                                    LEV06340
   DO 510 J = 2,NGM1                                               LEV06350
   T0 = V2(J)-V2(J-1)                                              LEV06360
   T1 = V2(J+1)-V2(J)                                             LEV06370
   G(J) = T1                                                        LEV06380
   IF (T0.LT.T1) G(J) = -T0                                       LEV06390
510 CONTINUE                                                       LEV06400
C                                                                    LEV06410
C   WRITE GOOD T-EIGENVALUES OUT TO FILE 3.                        LEV06420
C                                                                    LEV06430
   WRITE(3,520)NG,NDIS,MEV,N,SVSEED,MATNO,MULTOL,IB,BTOL         LEV06440
520 FORMAT(4I6,I12,I8,' = NG,NDIS,MEV,N,SVEED,MATNO'/           LEV06450
1 E20.12,I6,E13.4,' = MUTOL,INDEX MINIMAL BETA,BTOL'/           LEV06460
1' EV NO',1X,'TMULT',10X,'GOOD EIGENVALUE',7X,'TMINGAP',7X,'AMINGAP LEV06470
1')                                                                 LEV06480
C                                                                    LEV06490
   WRITE(3,530)(I,MP(I),V2(I),V1(I),G(I), I=1,NG)                LEV06500
530 FORMAT(2I6,E25.16,2E14.3)                                     LEV06510

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C                                                    LEV06520
C   IF CONVERGENCE FLAG ICONV.NE.1 AND NUMBER OF T-MATRICES           LEV06530
C   CONSIDERED TO DATE IS LESS THAN NUMBER ALLOWED, INCREMENT MEV.   LEV06540
C   AND LOOP BACK TO 210 TO REPEAT COMPUTATIONS.  RESTORE BETA(MEV+1).LEV06550
C                                                    LEV06560
C   BETA(MP1) = BETAM                                                    LEV06570
C                                                    LEV06580
C   IF (MMB.LT.NMEVS.AND.ICONV.NE.1) GO TO 180                         LEV06590
C                                                    LEV06600
C   END OF LOOP ON DIFFERENT SIZE T-MATRICES ALLOWED.                 LEV06610
C                                                    LEV06620
540 CONTINUE                                                            LEV06630
C                                                    LEV06640
C   IF(ISTOP.EQ.0) WRITE(6,550)                                         LEV06650
550 FORMAT(/' T-MATRICES (ALPHA AND BETA) ARE NOW AVAILABLE, TERMINATELEV06660
1')                                                                    LEV06670
C   IF (IHIS.EQ.1.AND.KMAX.NE.MOLD) WRITE(1,560)                       LEV06680
560 FORMAT(/' ABOVE ARE THE FOLLOWING VECTORS '/                        LEV06690
1 ' ALPHA(I), I = 1,KMAX'/                                           LEV06700
2 ' BETA(I), I = 1,KMAX+1'/                                           LEV06710
3 ' FINAL TWO LANCZOS VECTORS OF ORDER N FOR I = KMAX,KMAX+1'/       LEV06720
4 ' ALL VECTORS IN THIS FILE HAVE HEX FORMAT 4Z20 '/                 LEV06730
5 ' ----- END OF FILE 1 NEW ALPHA, BETA HISTORY-----'///)LEV06740
C                                                    LEV06750
C   IF (ISTOP.EQ.0) GO TO 640                                           LEV06760
C                                                    LEV06770
C   WRITE(3,570)                                                         LEV06780
570 FORMAT(/' ABOVE ARE COMPUTED GOOD T-EIGENVALUES'/                 LEV06790
1 ' NG = NUMBER OF GOOD T-EIGENVALUES COMPUTED'/                     LEV06800
2 ' NDIS = NUMBER OF COMPUTED DISTINCT EIGENVALUES OF T(1,MEV)'/     LEV06810
3 ' N = ORDER OF A,  MATNO = MATRIX IDENT'/                          LEV06820
4 ' MULTOL = T-MULTIPLICITY TOLERANCE FOR T-EIGENVALUES IN BISEC'/   LEV06830
4 ' TMULT IS THE T-MULTIPLICITY OF GOOD T-EIGENVALUE'/              LEV06840
5 ' TMULT = -1 MEANS SPURIOUS T-EIGENVALUE TOO CLOSE'/              LEV06850
6 ' DO NOT COMPUTE ERROR ESTIMATES FOR SUCH EIGENVALUES'/           LEV06860
7 ' AMINGAP = MINIMAL GAP BETWEEN THE COMPUTED A-EIGENVALUES'/      LEV06870
8 ' AMINGAP .LT. 0. MEANS MINIMAL GAP IS DUE TO LEFT-HAND GAP'/      LEV06880
9 ' TMINGAP= MINIMAL GAP W.R.T.  DISTINCT EIGENVALUES IN T(1,MEV)'/LEV06890
1 ' TMINGAP .LT. 0. MEANS MINGAP IS DUE TO SPURIOUS T-EIGENVALUE'/  LEV06900
2 ' ----- END OF FILE 3 GOODEIGENVALUES-----'///)LEV06910
C                                                    LEV06920
C   IF (IDIST.EQ.1) WRITE(11,580)                                       LEV06930
580 FORMAT(/' ABOVE ARE THE DISTINCT EIGENVALUES OF T(1,MEV).'/     LEV06940
2 ' THE FORMAT IS          T-MULTIPLICITY    T-EIGENVALUE  TMINGAP'/ LEV06950
3 '          THIS FORMAT IS REPEATED TWICE ON EACH LINE.'/          LEV06960
4 ' T-MULTIPLICITY = -1 MEANS THAT THE SUBROUTINE ISOEV HAS TAGGED'LEV06970
5/' THIS SIMPLE T-EIGENVALUE AS HAVING A VERY CLOSE SPURIOUS'/     LEV06980
6 ' T-EIGENVALUE SO THAT NO ERROR ESTIMATE WILL BE COMPUTED'/      LEV06990
7 ' FOR THAT EIGENVALUE IN SUBROUTINE INVERR.'/                     LEV07000
8 ' TMINGAP .LT. 0, TMINGAP IS DUE TO LEFT GAP .GT. 0, RIGHT GAP.'/LEV07010
9 ' EACH OF THE DISTINCT T-EIGENVALUE TABLES IS FOLLOWED'/        LEV07020
9 ' BY THE T-MULTIPLICITY PATTERN.'/                                LEV07030
1 ' NDIS = NUMBER OF COMPUTED DISTINCT EIGENVALUES OF T(1,MEV).'/   LEV07040
2 ' NG = NUMBER OF GOOD T-EIGENVALUES.  '/                          LEV07050
3 ' NISO = NUMBER OF ISOLATED GOOD T-EIGENVALUES.  '/              LEV07060

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4 ' NISO ALSO IS THE COUNT OF +1 ENTRIES IN T-MULTIPLICITY PATTERN.LEV07070
5 '/' ----- END OF FILE 11 DISTINCT T-EIGENVALUES-----'///LEV07080
6 )
C
IF(NISO.NE.0) WRITE(4,590)
590 FORMAT('/' ABOVE ARE THE ERROR ESTIMATES OBTAINED FOR THE ISOLATED LEV07120
1GOOD T-EIGENVALUES'/'
1' OBTAINED VIA INVERSE ITERATION IN THE SUBROUTINE INVERR.'/' LEV07140
1' ALL OTHER GOOD T-EIGENVALUES HAVE CONVERGED.'/' LEV07150
2' ERROR ESTIMATE = BETAM*ABS(UM)'/' LEV07160
2' WHERE BETAM = BETA(MEV+1) AND UM = U(MEV).'/' LEV07170
3' U = UNIT EIGENVECTOR OF T WHERE T*U = EV*U AND EV = ISOLATED GOOLEV07180
3D T-EIGENVALUE.'/' LEV07190
4' TMINGAP = GAP TO NEAREST DISTINCT EIGENVALUE OF T(1,MEV).'/' LEV07200
5' TMINGAP .LT. 0. MEANS MINGAP IS DUE TO A LEFT NEIGHBOR.'/' LEV07210
6' ERROR ESTIMATE L.T. 0 MEANS INVERSE ITERATION DID NOT CONVERGE'/'LEV07220
7' ----- END OF FILE 4 ERRINV -----'//) LEV07230
GO TO 640
C
600 CONTINUE
C
IBB = IABS(IBMEV)
IF (IBMEV.LT.0) WRITE(6,610) MEV,IBB,BETA(IBB)
610 FORMAT('/' PROGRAM TERMINATES BECAUSE MEV REQUESTED = ',I6,' IS .GTLEV07300
1',I6/' AT WHICH AN ABNORMALLY SMALL BETA = ' , E13.4,' OCCURRED'//)LEV07310
GO TO 640
C
620 IF (NDIS.EQ.0.AND.ISTOP.GT.0) WRITE(6,630)
630 FORMAT('/' INTERVALS SPECIFIED FOR BISECT DID NOT CONTAIN ANY T-EIGLEV07350
1ENVALUES'/' PROGRAM TERMINATES' )
C
640 CONTINUE
C
STOP
C-----END OF MAIN PROGRAM FOR LANCZOS EIGENVALUE COMPUTATIONS-----LEV07410
END
END

```

## 2.4 LEVEC: Main Program, Eigenvector Computations

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C-----LEVEC (EIGENVECTORS OF REAL SYMMETRIC MATRICES)-----LEV00010
C  Authors:  Jane Cullum and Ralph A. Willoughby (Deceased)      LEV00020
C              Los Alamos National Laboratory                    LEV00030
C              Los Alamos, New Mexico 87544                    LEV00040
C                                                                 LEV00050
C              E-mail:  cullumj@lanl.gov                        LEV00060
C                                                                 LEV00070
C  These codes are copyrighted by the authors.  These codes    LEV00080
C  and modifications of them or portions of them are NOT to be LEV00090
C  incorporated into any commercial codes or used for any other LEV00100
C  commercial purposes such as consulting for other companies,  LEV00110
C  without legal agreements with the authors of these Codes.   LEV00120
C  If these Codes or portions of them are used in other scientific or LEV00130
C  engineering research works the names of the authors of these codes LEV00140
C  and appropriate references to their written work are to be   LEV00150
C  incorporated in the derivative works.                        LEV00160
C                                                                 LEV00170
C  This header is not to be removed from these codes.          LEV00180
C                                                                 LEV00190
C              REFERENCE: Cullum and Willoughby, Chapters 1,2,3,4 LEV00191
C              Lanczos Algorithms for Large Symmetric Eigenvalue Computations LEV00192
C              VOL. 1 Theory. Republished as Volume 41 in SIAM CLASSICS in LEV00193
C              Applied Mathematics, 2002. SIAM Publications,    LEV00194
C              Philadelphia, PA. USA                            LEV00195
C                                                                 LEV00196
C                                                                 LEV00197
C                                                                 LEV00200
C  CONTAINS MAIN PROGRAM FOR COMPUTING AN EIGENVECTOR CORRESPONDING LEV00210
C  TO EACH OF A SET OF EIGENVALUES WHICH HAVE BEEN COMPUTED    LEV00220
C  ACCURATELY BY THE CORRESPONDING LANCZOS EIGENVALUE PROGRAM  LEV00230
C  (LEVAL) FOR REAL SYMMETRIC MATRICES.  THIS PROGRAM COULD BE LEV00240
C  MODIFIED TO COMPUTE ADDITIONAL EIGENVECTORS FOR ANY EIGENVALUE LEV00250
C  WHICH IS A MULTIPLE EIGENVALUE OF THE GIVEN A-MATRIX.  THE LEV00260
C  AMOUNT OF ADDITIONAL COMPUTATION REQUIRED WOULD DEPEND UPON LEV00270
C  THE GIVEN A-MATRIX AND UPON WHAT PART OF THE SPECTRUM OF   LEV00280
C  A IS INVOLVED.                                             LEV00290
C                                                                 LEV00300
C  THE LANCZOS EIGENVECTOR COMPUTATIONS ASSUME THAT EACH      LEV00310
C  EIGENVALUE THAT IS BEING CONSIDERED HAS CONVERGED AS AN    LEV00320
C  EIGENVALUE OF THE LANCZOS TRIDIAGONAL MATRICES.           LEV00330
C                                                                 LEV00340
C  PFORT VERIFIER IDENTIFIED THE FOLLOWING NONPORTABLE        LEV00350
C  CONSTRUCTIONS                                              LEV00360
C                                                                 LEV00370
C  1.  DATA/MACHEP/ STATEMENT                                LEV00380
C  2.  ALL READ(5,*) STATEMENTS (FREE FORMAT)                 LEV00390
C  3.  FORMAT(20A4) USED WITH THE EXPLANATORY HEADER, EXPLAN  LEV00400
C  4.  HEXADECIMAL FORMAT (4Z20) USED IN ALPHA/BETA FILES 1 AND 2. LEV00410
C                                                                 LEV00420
C  IMPORTANT NOTE:  THIS PROGRAM ALLOWS ENLARGEMENT OF THE ALPHA, LEV00430
C  BETA ARRAYS.  IN PARTICULAR, IF ANY ONE OF THE EIGENVALUES LEV00440
C  SUPPLIED IS T-SIMPLE AND NOT CLOSE TO A SPURIOUS EIGENVALUE, LEV00450

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C THE PROGRAM REQUIRES THAT KMAX BE AT LEAST 11*MEV/8 + 12. IF LEV00460
C KMAX IS NOT THIS LARGE, THEN THE PROGRAM RESETS KMAX TO THIS LEV00470
C SIZE AND EXTENDS THE ALPHA, BETA HISTORY IF REQUIRED. LEV00480
C THUS, THE DIMENSIONS OF THE ALPHA AND BETA ARRAYS MUST BE LEV00490
C LARGE ENOUGH TO ALLOW FOR THIS POSSIBILITY. LEV00500
C REMEMBER THAT THE BETA ARRAY, BETA(J), IS SUCH THAT LEV00510
C J = 1, ..., KMAX+1. SO IF THE KMAX USED BY THE PROGRAM LEV00520
C IS TO BE 3000, THEN BETA MUST BE OF LENGTH AT LEAST 3001. LEV00530
C LEV00540
C-----LEV00550
DOUBLE PRECISION ALPHA(5000),BETA(5001) LEV00560
DOUBLE PRECISION V1(5000),V2(5000) LEV00570
DOUBLE PRECISION RITVEC(30000),TVEC(30000),GOODEV(50),EVNEW(50) LEV00580
DOUBLE PRECISION EVAL,EVALN,TOLN,TTOL,ERTOL,ALFA,BATA LEV00590
DOUBLE PRECISION MULTOL,SCALEO,STUTOL,BTOL,LB,UB LEV00600
DOUBLE PRECISION ONE,ZERO,MACHEP,EPSM,TEMP,SUM,ERRMIN,BKMIN LEV00610
DOUBLE PRECISION RELTOL,ERROR,TERROR,TLAST(50) LEV00620
REAL G(10000),AMINGP(50),TMINGP(50),EXPLAN(20) LEV00630
REAL TERR(50),ERR(50),ERRDGP(50),RNORM(50),TBETA(50) LEV00640
INTEGER MP(50),M1(50),M2(50),MA(50),ML(50),MINT(50),MFIN(50) LEV00650
INTEGER SVSEED,SVSOLD,RHSEED,IDELTA(50) LEV00660
INTEGER MBOUND,NTVCON,SVTVEC,TVSTOP,LVCONT,ERCONT,TFLAG LEV00670
DOUBLE PRECISION FINPRO LEV00680
DOUBLE PRECISION DABS,DMAX1,DSQRT,DFLOAT LEV00690
REAL ABS LEV00700
INTEGER IABS LEV00710
C-----LEV00720
EXTERNAL CMATV LEV00730
DATA MACHEP/Z3410000000000000/ LEV00740
EPSM = 2.D0*MACHEP LEV00750
C-----LEV00760
C LEV00770
C ARRAYS MUST BE DIMENSIONED AS FOLLOWS: LEV00780
C 1. ALPHA: >= KMAXN, BETA: >= (KMAXN+1) WHERE KMAXN, THE LEV00790
C LARGEST SIZE T-MATRIX CONSIDERED BY THE PROGRAM, LEV00800
C IS THE LARGER OF THE SIZE OF THE ALPHA, BETA HISTORY LEV00810
C PROVIDED ON FILE 2 (IF ANY ) AND THE SIZE WHICH THE LEV00820
C PROGRAM SPECIFIES INTERNALLY, THIS LATTER IS ALWAYS LEV00830
C < = 11*MEV / 8 + 12, WHERE MEV IS THE SIZE LEV00840
C T-MATRIX THAT WAS USED IN THE CORRESPONDING EIGENVALUE LEV00850
C COMPUTATIONS. LEV00860
C 2. V1: >= MAX(N,KMAX) LEV00870
C 3. V2: >= N LEV00880
C 4. G: >= MAX(N,KMAX) LEV00890
C 5. RITVEC: >= N*NGOOD, WHERE NGOOD IS NUMBER OF EIGENVALUES LEV00900
C SUPPLIED TO THIS PROGRAM. LEV00910
C 6. TVEC: >= CUMULATIVE LENGTH OF ALL THE T-EIGENVECTORS LEV00920
C NEEDED TO GENERATE THE DESIRED RITZ VECTORS. AN EDUCATED LEV00930
C GUESS AT AN APPROPRIATE LENGTH CAN BE OBTAINED BY RUNNING THE LEV00940
C PROGRAM WITH THE FLAG MBOUND = 1 AND MULTIPLYING THE LEV00950
C RESULTING SIZE BY 5/4. LEV00960
C 7. GOODEV, AMINGP, TMINGP, TERR, ERR, ERRGDP, RNORM, TBETA, LEV00970
C TLAST, EVNEW, MP, MA, M1, M2, MINT, MFIN AND IDELTA ALL MUST LEV00980
C BE >= NGOOD. LEV00990
C LEV01000

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C-----LEV01010
C   OUTPUT HEADER                                LEV01020
C   WRITE(6,10)                                  LEV01030
10  FORMAT(/' LANCZOS EIGENVECTOR PROCEDURE FOR REAL SYMMETRIC MATRICELEV01040
   1S'/)                                         LEV01050
C                                               LEV01060
C   SET PROGRAM PARAMETERS                       LEV01070
C   USER MUST NOT MODIFY SCALE0                LEV01080
C   SCALE0 = 5.0D0                              LEV01090
C   ZERO = 0.0D0                                LEV01100
C   ONE = 1.0D0                                  LEV01110
C   MPMIN = -1000                               LEV01120
C   SET CONVERGENCE CRITERION FOR T-EIGENVECTORS. LEV01130
C   ERTOL = 1.D-10                              LEV01140
C                                               LEV01150
C   READ USER-SPECIFIED PARAMETER FROM INPUT FILE 5 (FREE FORMAT) LEV01160
C                                               LEV01170
C   READ USER-PROVIDED HEADER FOR RUN           LEV01180
C   READ(5,20) EXPLAN                            LEV01190
C   WRITE(6,20) EXPLAN                           LEV01200
20  FORMAT(20A4)                                LEV01210
C                                               LEV01220
C   READ IN THE MAXIMUM PERMISSIBLE DIMENSIONS FOR THE TVEC ARRAY LEV01230
C   (MDIMTV), FOR THE RITVEC ARRAY (MDIMRV), AND FOR THE BETA LEV01240
C   ARRAY (MBETA).                               LEV01250
C   READ(5,20) EXPLAN                            LEV01260
C   READ(5,*) MDIMTV, MDIMRV, MBETA             LEV01270
C                                               LEV01280
C   READ IN RELATIVE TOLERANCE (RELTOL) USED IN DETERMINING LEV01290
C   APPROPRIATE SIZES FOR THE T-MATRICES TO BE USED IN THE RITZ LEV01300
C   VECTOR COMPUTATIONS.                       LEV01310
C   READ(5,20) EXPLAN                            LEV01320
C   READ(5,*) RELTOL                             LEV01330
C                                               LEV01340
C   SET FLAGS TO 0 OR 1:                        LEV01350
C   MBOUND = 1: PROGRAM TERMINATES AFTER COMPUTING 1ST GUESSES LEV01360
C   ON APPROPRIATE T-SIZES FOR USE IN THE RITZ VECTOR LEV01370
C   COMPUTATIONS                                LEV01380
C   NTVCON = 0: PROGRAM TERMINATES IF THE TVEC ARRAY IS NOT LEV01390
C   LARGE ENOUGH TO HOLD ALL THE T-EIGENVECTORS REQUIRED. LEV01400
C   SVTVEC = 0: THE T-EIGENVECTORS ARE NOT WRITTEN TO FILE 11 LEV01410
C   UNLESS TVSTOP = 1                           LEV01420
C   SVTVEC = 1: WRITE THE T-EIGENVECTORS TO FILE 11. LEV01430
C   TVSTOP = 1: PROGRAM TERMINATES AFTER COMPUTING THE LEV01440
C   T-EIGENVECTORS                              LEV01450
C   LVCONT = 0: PROGRAM TERMINATES IF THE NUMBER OF T-EIGENVECTORS LEV01460
C   COMPUTED IS NOT EQUAL TO THE NUMBER OF RITZ LEV01470
C   VECTORS REQUESTED.                          LEV01480
C   ERCONT = 0: MEANS FOR ANY GIVEN EIGENVALUE, A RITZ VECTOR LEV01490
C   WILL NOT BE COMPUTED FOR THAT EIGENVALUE UNLESS LEV01500
C   A T-EIGENVECTOR HAS BEEN IDENTIFIED WITH A LAST LEV01510
C   COMPONENT WHICH SATISFIES THE SPECIFIED LEV01520
C   CONVERGENCE CRITERION.                     LEV01530
C   ERCONT = 1: MEANS FOR ANY GIVEN EIGENVALUE, A RITZ VECTOR LEV01540
C   WILL BE COMPUTED. IF A T-EIGENVECTOR CANNOT LEV01550

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C          BE IDENTIFIED WHICH SATISFIES THE LAST          LEV01560
C          COMPONENT CRITERION, THEN THE PROGRAM WILL      LEV01570
C          USE THE T-VECTOR THAT CAME CLOSEST TO          LEV01580
C          SATISFYING THE CRITERION.                     LEV01590
C  IWRITE = 1: EXTENDED OUTPUT OF INTERMEDIATE COMPUTATIONS LEV01600
C              IS WRITTEN TO FILE 6                      LEV01610
C  IREAD = 0:  ALPHA/BETA FILE IS REGENERATED.           LEV01620
C  IREAD = 1:  ALPHA/BETA FILE USED IN EIGENVALUE COMPUTATIONS LEV01630
C              IS READ IN AND EXTENDED IF NECESSARY.  IN BOTH LEV01640
C              CASES IREAD = 0 OR 1, THE LANCZOS VECTORS ARE LEV01650
C              ALWAYS REGENERATED FOR THE RITZ VECTOR    LEV01660
C              COMPUTATIONS                              LEV01670
C                                                      LEV01680
C  READ(5,20) EXPLAN                                     LEV01690
C  READ(5,*) MBOUND,NTVCON,SVTVEC,IREAD                 LEV01700
C                                                      LEV01710
C  READ(5,20) EXPLAN                                     LEV01720
C  READ(5,*) TVSTOP,LVCONT,ERCONT,IWRITE               LEV01730
C  IF (TVSTOP.EQ.1) SVTVEC = 1                          LEV01740
C                                                      LEV01750
C  READ IN SEED (RHSEED) FOR GENERATING RANDOM STARTING VECTOR LEV01760
C  FOR INVERSE ITERATION ON THE T-MATRICES.            LEV01770
C  READ(5,20) EXPLAN                                     LEV01780
C  READ(5,*) RHSEED                                     LEV01790
C                                                      LEV01800
C  READ IN MATNO = MATRIX/RUN IDENTIFICATION NUMBER AND LEV01810
C  N = ORDER OF A-MATRIX                                LEV01820
C  READ(5,20) EXPLAN                                     LEV01830
C  READ(5,*) MATNO,N                                   LEV01840
C                                                      LEV01850
C-----LEV01860
C  INITIALIZE THE ARRAYS FOR THE USER-SPECIFIED MATRIX   LEV01870
C  AND PASS THE STORAGE LOCATIONS OF THESE ARRAYS TO THE LEV01880
C  MATRIX-VECTOR MULTIPLY SUBROUTINE CMATV.             LEV01890
C                                                      LEV01900
C  CALL USPEC(N,MATNO)                                  LEV01910
C                                                      LEV01920
C-----LEV01930
C  MASK UNDERFLOW AND OVERFLOW                          LEV01940
C  CALL MASK                                             LEV01950
C                                                      LEV01960
C-----LEV01970
C  WRITE RUN PARAMETERS OUT TO FILE 6                   LEV01980
C                                                      LEV01990
C  WRITE(6,30) MATNO,N                                  LEV02000
C  30 FORMAT(/' MATRIX IDENTIFICATION NO. = ',I10,' ORDER OF A = ',I5) LEV02010
C                                                      LEV02020
C  WRITE(6,40) MBOUND,NTVCON,SVTVEC,IREAD              LEV02030
C  40 FORMAT(/3X,'MBOUND',3X,'NTVCON',3X,'SVTVEC',3X,'IREAD'/3I9,I8) LEV02040
C                                                      LEV02050
C  WRITE(6,50) TVSTOP,LVCONT,ERCONT,IWRITE            LEV02060
C  50 FORMAT(/3X,'TVSTOP',3X,'LVCONT',3X,'ERCONT',3X,'IWRITE'/4I9) LEV02070
C                                                      LEV02080
C  WRITE(6,60) MDIMTV,MDIMRV,MBETA                     LEV02090
C  60 FORMAT(/3X,'MDIMTV',3X,'MDIMRV',3X,'MBETA'/2I9,I8) LEV02100

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C                                                    LEV02110
      WRITE(6,70) RELTOL,RHSEED                        LEV02120
70  FORMAT(/7X,'RELTOL',3X,'RHSEED'/E13.4,I9)        LEV02130
C                                                    LEV02140
C                                                    LEV02150
C  FROM FILE 3 READ IN THE NUMBER OF EIGENVALUES (NGOOD) FOR WHICH LEV02160
C  EIGENVECTORS ARE REQUESTED, THE ORDER (MEV) OF THE LANCZOS      LEV02170
C  TRIDIAGONAL MATRIX USED IN COMPUTING THESE EIGENVALUES, THE     LEV02180
C  ORDER (NOLD) OF THE USER-SPECIFIED MATRIX USED IN THE EIGENVALUE LEV02190
C  COMPUTATIONS, THE SEED (SVSEED) USED FOR GENERATING THE STARTING LEV02200
C  VECTOR THAT WAS USED IN THOSE LANCZOS EIGENVALUE COMPUTATIONS,   LEV02210
C  AND THE MATRIX/RUN IDENTIFICATION NUMBER (MATOLD) USED IN THOSE  LEV02220
C  COMPUTATIONS. ALSO READ IN THE NUMBER (NDIS) OF DISTINCT        LEV02230
C  EIGENVALUES OF T(1,MEV) THAT WERE COMPUTED BUT THIS VALUE IS    LEV02240
C  NOT USED IN THE EIGENVECTOR COMPUTATIONS.                      LEV02250
C                                                    LEV02260
      READ(3,80) NGOOD,NDIS,MEV,NOLD,SVSEED,MATOLD    LEV02270
80  FORMAT(4I6,I12,I8)                                       LEV02280
C                                                    LEV02290
C  READ IN THE T-MULTIPLICITY TOLERANCE USED IN THE BISEC SUBROUTINE LEV02300
C  DURING THE COMPUTATION OF THE GIVEN EIGENVALUES.                LEV02310
C  ALSO READ IN THE FLAG IB. IF IB < 0, THEN SOME BETA(I) IN THE   LEV02320
C  T-MATRIX FILE PROVIDED ON FILE 2 FAILED THE ORTHOGONALITY      LEV02330
C  TEST IN THE TNORM SUBROUTINE. USER SHOULD NOTE THAT THIS VECTOR LEV02340
C  PROGRAM PROCEEDS INDEPENDENTLY OF THE SIZE OF THE BETA USED.   LEV02350
C                                                    LEV02360
      READ(3,90) MULTOL,IB,BTOL                        LEV02370
90  FORMAT(E20.12,I6,E13.4)                               LEV02380
C                                                    LEV02390
      TEMP = DFLOAT(MEV+1000)                          LEV02400
      TTOL = MULTOL/TEMP                               LEV02410
      WRITE(6,100) MULTOL,TTOL                         LEV02420
100 FORMAT('/ T-MULTIPLICITY TOLERANCE USED IN THE EIGENVALUE COMPUTATLEV02430
      IONS WAS',E13.4/' SCALED MACHINE EPSILON IS',E13.4)        LEV02440
C                                                    LEV02450
C  CONTINUE WRITE TO FILE 6 OF THE PARAMETERS FOR THIS RUN       LEV02460
C                                                    LEV02470
      WRITE(6,110)NGOOD,NDIS,MEV,NOLD,MATOLD,SVSEED,MULTOL,IB,BTOL LEV02480
110 FORMAT('/ EIGENVALUES SUPPLIED ARE READ IN FROM FILE 3'/' FILE 3 LEV02490
      1HEADER IS'/4X,'NG',2X,'NDIS',3X,'MEV',2X,'NOLD',2X,'MATOLD',4X, LEV02500
      1'SVSEED',6X,'MULTOL',6X,'IB',9X,'BTOL'/4I6,I8,I10,E12.3,I8,E13.4/)LEV02510
C                                                    LEV02520
C  IS THE ARRAY RITVEC LONG ENOUGH TO HOLD ALL OF THE DESIRED     LEV02530
C  RITZ VECTORS (APPROXIMATE EIGENVECTORS)?                       LEV02540
      NMAX = NGOOD*N                                    LEV02550
      IF(MBOUND.NE.0) GO TO 120                          LEV02560
      IF(TVSTOP.NE.1.AND.NMAX.GT.MDIMRV) GO TO 1310      LEV02570
C                                                    LEV02580
C  CHECK THAT THE ORDER N AND THE MATRIX IDENTIFICATION NUMBER     LEV02590
C  MATNO SPECIFIED BY THE USER AGREE WITH THOSE READ IN FROM     LEV02600
C  FILE 3.                                                         LEV02610
120 ITEM = (NOLD-N)**2+(MATOLD-MATNO)**2               LEV02620
      IF (ITEM.NE.0) GO TO 1330                          LEV02630
C                                                    LEV02640
C  READ IN FROM FILE 3, THE T-MULTIPLICITIES OF THE EIGENVALUES  LEV02650

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C   WHOSE EIGENVECTORS ARE TO BE COMPUTED, THE VALUES OF THESE          LEV02660
C   EIGENVALUES AND THEIR MINIMAL GAPS AS EIGENVALUES OF THE              LEV02670
C   USER-SPECIFIED MATRIX AND AS EIGENVALUES OF THE T-MATRIX.           LEV02680
C                                                                           LEV02690
      READ(3,20) EXPLAN                                                    LEV02700
      READ(3,130) (MP(J),GOODEV(J),TMINGP(J),AMINGP(J), J=1,NGOOD)        LEV02710
130  FORMAT(6X,I6,E25.16,2E14.3)                                          LEV02720
C                                                                           LEV02730
      WRITE(6,140) (J,GOODEV(J),MP(J),TMINGP(J),AMINGP(J), J=1,NGOOD)    LEV02740
140  FORMAT(/' EIGENVALUES READ IN, T-MULTIPLICITIES, T-GAPS AND A-GAPS    LEV02750
      1  '/4X,' J ',5X,'GOOD EIGENVALUE',5X,'MULT',4X,' TMINGAP ',4X,     LEV02760
      1  ' AMINGAP '/(I6,E25.16,I4,2E15.4))                                LEV02770
C                                                                           LEV02780
C   READ IN ERROR ESTIMATES                                              LEV02790
      WRITE(6,150) MEV,SVSEED                                             LEV02800
150  FORMAT(/' THESE EIGENVALUES WERE COMPUTED USING A T-MATRIX OF        LEV02810
      10ORDER ',I5/' AND SEED FOR RANDOM NUMBER GENERATOR =' ,I12)        LEV02820
C   CHECK WHETHER OR NOT THERE ARE ANY T-ISOLATED EIGENVALUES IN        LEV02830
C   THE EIGENVALUES PROVIDED                                             LEV02840
      DO 160 J=1,NGOOD                                                    LEV02850
      IF(MP(J).EQ.1) GO TO 170                                            LEV02860
160  CONTINUE                                                            LEV02870
      GO TO 190                                                            LEV02880
170  READ(4,20) EXPLAN                                                    LEV02890
      READ(4,20) EXPLAN                                                    LEV02900
      READ(4,20) EXPLAN                                                    LEV02910
      READ(4,180) NISO                                                    LEV02920
180  FORMAT(18X,I6)                                                       LEV02930
      READ(4,20) EXPLAN                                                    LEV02940
      READ(4,20) EXPLAN                                                    LEV02950
      READ(4,20) EXPLAN                                                    LEV02960
190  DO 220 J=1,NGOOD                                                    LEV02970
      ERR(J) = 0.DO                                                       LEV02980
      IF(MP(J).NE.1) GO TO 220                                            LEV02990
      READ(4,200) EVAL, ERR(J)                                             LEV03000
200  FORMAT(10X,E25.16,E14.3)                                             LEV03010
      IF(DABS(EVAL - GOODEV(J)).LT.1.D-10) GO TO 220                     LEV03020
      WRITE(6,210) EVAL,GOODEV(J)                                         LEV03030
210  FORMAT(' PROBLEM WITH READ IN OF ERROR ESTIMATES'/' EIGENVALUE RE    LEV03040
      1D IN',E20.12,' DOES NOT MATCH GOODEV(J) =' /E20.12)             LEV03050
      GO TO 1550                                                           LEV03060
C                                                                           LEV03070
220  CONTINUE                                                            LEV03080
C                                                                           LEV03090
      WRITE(6,230) (J,GOODEV(J),ERR(J), J=1,NGOOD)                       LEV03100
230  FORMAT(' ERROR ESTMATES =' /4X,' J ',5X,'EIGENVALUE',10X,' ESTIMATE  LEV03110
      1'/(I6,E20.12,E14.3))                                              LEV03120
C                                                                           LEV03130
      IF(IREAD.EQ.0) GO TO 330                                            LEV03140
C                                                                           LEV03150
C   READ IN THE SIZE OF THE T-MATRIX PROVIDED ON FILE 2. READ IN        LEV03160
C   THE ORDER OF THE USER-SPECIFIED MATRIX , THE SEED FOR THE          LEV03170
C   RANDOM NUMBER GENERATOR, AND THE MATRIX/TEST IDENTIFICATION         LEV03180
C   NUMBER THAT WERE USED IN THE LANCZOS EIGENVALUE COMPUTATIONS.       LEV03190
C   THESE ARE USED IN A CONSISTENCY CHECK                                LEV03200

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C      IF FLAG IREAD = 0 REGENERATE ALPHA, BETA                                LEV03210
C                                                                                   LEV03220
      READ(2,240) KMAX,NOLD,SVSOLD,MATOLD                                       LEV03230
240  FORMAT(2I6,I12,I8)                                                         LEV03240
C                                                                                   LEV03250
      WRITE(6,250) KMAX,NOLD,SVSOLD,MATOLD                                       LEV03260
250  FORMAT(/' READ IN THE T-MATRICES STORED ON FILE 2'/' FILE 2 HEADERLEV03270
      1 IS'/2X,'KMAX',2X,'NOLD',6X,'SVSOLD',2X,'MATOLD'/2I6,I12,I8/)           LEV03280
C                                                                                   LEV03290
C      CHECK THAT THE ORDER, THE MATRIX/TEST IDENTIFICATION NUMBER              LEV03300
C      AND THE SEED FOR THE RANDOM NUMBER GENERATOR USED IN THE                 LEV03310
C      LANZOS COMPUTATIONS THAT GENERATED THE ALPHA,BETA FILE                  LEV03320
C      BEING USED AGREE WITH WHAT THE USER HAS SPECIFIED.                    LEV03330
C      IF (NOLD.NE.N.OR.MATOLD.NE.MATNO.OR.SVSOLD.NE.SVSEED) GO TO 1350        LEV03340
C                                                                                   LEV03350
      KMAX1 = KMAX + 1                                                           LEV03360
C                                                                                   LEV03370
C      READ IN THE T-MATRICES FROM FILE 2.  THESE ARE USED TO GENERATE          LEV03380
C      THE T-EIGENVECTORS THAT WILL BE USED IN THE RITZ VECTOR                 LEV03390
C      COMPUTATIONS.  HISTORY MUST BE STORED IN MACHINE FORMAT                 LEV03400
C      ((4Z20) FOR IBM/3081)                                                    LEV03410
C                                                                                   LEV03420
      READ(2,260) (ALPHA(J), J=1,KMAX)                                           LEV03430
      READ(2,260) (BETA(J), J=1,KMAX1)                                           LEV03440
260  FORMAT(4Z20)                                                                LEV03450
C                                                                                   LEV03460
      READ(2,260) (V1(J), J=1,N)                                                 LEV03470
      READ(2,260) (V2(J), J=1,N)                                                 LEV03480
C                                                                                   LEV03490
C      KMAX MAY BE ENLARGED IF THE SIZE AT WHICH THE EIGENVALUE                LEV03500
C      COMPUTATIONS WERE PERFORMED IS ESSENTIALLY KMAX AND                    LEV03510
C      THERE IS AT LEAST ONE EIGENVALUE THAT IS T-SIMPLE AND                  LEV03520
C      T-ISOLATED, IN THE SENSE THAT IF ITS NEAREST NEIGHBOR IS TOO           LEV03530
C      CLOSE THAT NEIGHBOR IS A 'GOOD' T-EIGENVALUE.                          LEV03540
      DO 270 J = 1,NGOOD                                                         LEV03550
      IF(MP(J).EQ.1) GO TO 290                                                    LEV03560
270  CONTINUE                                                                    LEV03570
      WRITE(6,280)                                                                LEV03580
280  FORMAT(/' ALL EIGENVALUES USED ARE T-MULTIPLE OR CLOSE TO SPURIOUSLEV03590
      1 T-EIGENVALUES'/' SO KMAX IS NOT INCREASED')                             LEV03600
      IF(KMAX.LT.MEV) GO TO 1370                                                 LEV03610
      GO TO 310                                                                    LEV03620
C                                                                                   LEV03630
290  KMAXN= 11*MEV/8 + 12                                                         LEV03640
      IF(MBETA.LE.KMAXN) GO TO 1530                                              LEV03650
      IF(KMAX.GE.KMAXN ) GO TO 310                                               LEV03660
      WRITE(6,300) KMAX, KMAXN                                                   LEV03670
300  FORMAT(' ENLARGE KMAX FROM ',I6,' TO ',I6)                                 LEV03680
      MOLD1 = KMAX + 1                                                           LEV03690
      KMAX = KMAXN                                                               LEV03700
      GO TO 380                                                                    LEV03710
C                                                                                   LEV03720
310  WRITE(6,320) KMAX                                                           LEV03730
320  FORMAT(/' T-MATRICES HAVE BEEN READ IN FROM FILE 2'/' THE LARGEST LEV03740
      1SIZE T-MATRIX ALLOWED IS',I6/)                                           LEV03750

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C                                                    LEV03760
      IF(IREAD.EQ.1) GO TO 400                        LEV03770
C                                                    LEV03780
C      REGENERATE THE ALPHA AND BETA                LEV03790
C                                                    LEV03800
330 MOLD1 = 1                                        LEV03810
C                                                    LEV03820
      DO 340 J = 1,NGOOD                             LEV03830
      IF(MP(J).EQ.1) GO TO 360                       LEV03840
340 CONTINUE                                        LEV03850
      KMAX = MEV + 12                                LEV03860
      WRITE(6,350) KMAX                              LEV03870
350 FORMAT(/' ALL EIGENVALUES FOR WHICH EIGENVECTORS ARE TO BE COMPUTE
1D ARE EITHER T-MULTIPLE OR CLOSE TO'/' A SPURIOUS T-EIGENVALUE. TH
1EREFORE SET KMAX = MEV + 12 = ',I7)              LEV03900
      GO TO 380                                      LEV03910
C                                                    LEV03920
360 KMAXN = 11*MEV/8 + 12                          LEV03930
      IF(MBETA.LE.KMAXN) GO TO 1530                 LEV03940
      WRITE(6,370) KMAXN                           LEV03950
370 FORMAT(' SET KMAX EQUAL TO ',I6)              LEV03960
      KMAX = KMAXN                                  LEV03970
C                                                    LEV03980
380 WRITE(6,390) MOLD1,KMAX                        LEV03990
390 FORMAT(/' LANCZS SUBROUTINE GENERATES ALPHA(J), BETA(J+1), J =',
1 I6,' TO ', I6/)                                LEV04000
C                                                    LEV04010
C                                                    LEV04020
C-----LEV04030
C                                                    LEV04040
C      IIX = SVSEED                                 LEV04050
      CALL LANCZS(CMATV,ALPHA,BETA,V1,V2,G,KMAX,MOLD1,N,IIX) LEV04060
C                                                    LEV04070
C-----LEV04080
C                                                    LEV04090
400 CONTINUE                                        LEV04100
C                                                    LEV04110
C      THE SUBROUTINE STURMI DETERMINES THE SMALLEST SIZE T-MATRIX FOR
C      WHICH THE EIGENVALUE IN QUESTION IS A T-EIGENVALUE (TO WITHIN A
C      GIVEN TOLERANCE) AND IF POSSIBLE THE SMALLEST SIZE T-MATRIX
C      FOR WHICH IT IS A DOUBLE T-EIGENVALUE (TO WITHIN THE SAME
C      TOLERANCE). THE SIZE T-MATRIX USED IN THE RITZ VECTOR
C      COMPUTATIONS IS THEN DETERMINED BY LOOPING ON SIZE OF THE
C      T-EIGENVECTORS STARTING WITH A T-SIZE DETERMINED FROM THE
C      OUTPUT FROM STURMI.                         LEV04190
C                                                    LEV04200
C                                                    LEV04210
C      STUTOL = SCALEO*MULTOL                       LEV04220
      IF(IWRITE.EQ.1) WRITE(6,410)                 LEV04230
410 FORMAT(' FROM STURMI')                        LEV04240
      DO 450 J = 1,NGOOD                             LEV04250
      EVAL = GOODEV(J)                              LEV04260
C      COMPUTE THE TOLERANCES USED BY STURMI TO DETERMINE AN INTERVAL
C      CONTAINING THE EIGENVALUE EVAL.             LEV04280
      TEMP = DABS(EVAL)*RELTOL                      LEV04290
      TOLN = DMAX1(TEMP,STUTOL)                    LEV04300

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C                                                    LEV04310
C-----LEV04320
C                                                    LEV04330
      CALL STURMI(ALPHA,BETA,EVAL,TOLN,EPSM,KMAX,MK1,MK2,IC,IWRITE)  LEV04340
C                                                    LEV04350
C-----LEV04360
C                                                    LEV04370
C  STORE THE COMPUTED ORDERS OF T-MATRICES FOR LATER PRINTOUT      LEV04380
      M1(J) = MK1                                                    LEV04390
      M2(J) = MK2                                                    LEV04400
      ML(J) = (MK1 + 3*MK2)/4                                         LEV04410
      IF(MK2.EQ.KMAX) ML(J) = KMAX                                     LEV04420
C                                                    LEV04430
      IF(IC.GT.0) GO TO 430                                           LEV04440
C  IC = 0 MEANS THERE WAS NO EIGENVALUE IN THE DESIGNATED INTERVAL  LEV04450
C  BY T-SIZE KMAX. THIS MEANS THAT THE EIGENVALUE PROVIDED HAS     LEV04460
C  NOT YET CONVERGED SO ITS EIGENVECTOR WILL NOT BE COMPUTED.     LEV04470
      WRITE(6,420) J,GOODEV(J),MK1,MK2                               LEV04480
420  FORMAT(I6,'TH EIGENVALUE',E20.12,' HAS NOT CONVERGED '/
1' SO DO NOT COMPUTE ANY T-EIGENVECTOR OR RITZ VECTOR FOR IT'
1/' MK1 AND MK2 FOR THIS EIGENVALUE WERE',2I6)                     LEV04500
      MP(J) = MPMIN                                                  LEV04520
      MA(J) = -2*KMAX                                                 LEV04530
      GO TO 450                                                       LEV04540
C  COMPUTE AN APPROPRIATE SIZE T-MATRIX FOR THE GIVEN EIGENVALUE.  LEV04550
430  IF(M2(J).EQ.KMAX) GO TO 440                                       LEV04560
C  M1 AND M2 WERE BOTH DETERMINED                                    LEV04570
      MA(J) = (3*M1(J) + M2(J))/4 + 1                                 LEV04580
      GO TO 450                                                       LEV04590
C  M2 NOT DETERMINED                                               LEV04600
440  MA(J) = (5*M1(J))/4 + 1                                           LEV04610
C                                                    LEV04620
450  CONTINUE                                                         LEV04630
C                                                    LEV04640
      IF (IWRITE.EQ.1) WRITE(6,460) (MA(JJ), JJ=1,NGOOD)           LEV04650
460  FORMAT(/' 1ST GUESS AT APPROPRIATE SIZE T-MATRICES'/
1 ' ACTUAL VALUES WILL PROBABLY BE 1/4 AGAIN AS MUCH'/(13I6))    LEV04670
C                                                    LEV04680
C  PRINT OUT TO FILE 10 1ST GUESSES AT SIZES OF THE T-MATRICES TO  LEV04690
C  BE USED IN THE EIGENVECTOR COMPUTATIONS.                       LEV04700
C  PROGRAM LOOPS ON T-SIZE TO DETERMINE APPROPRIATE SIZE T-MATRIX. LEV04710
      WRITE(10,470) N,KMAX                                           LEV04720
470  FORMAT(2I8,' = ORDER OF USER MATRIX AND MAX ORDER OF T(1,MEV)') LEV04730
C                                                    LEV04740
      WRITE(10,480)                                                  LEV04750
480  FORMAT(/' 1ST GUESS AT APPROPRIATE SIZE T-MATRICES'/
1 ' ACTUAL VALUES WILL PROBABLY BE 1/4 AGAIN AS MUCH'//)        LEV04770
C                                                    LEV04780
      WRITE(10,490)                                                  LEV04790
490  FORMAT(4X,'J',4X,'A-EIGENVALUE',4X,'M1(J)',1X,'M2(J)',1X,'MA(J)') LEV04800
C                                                    LEV04810
      WRITE(10,500) (J,GOODEV(J),M1(J),M2(J), MA(J), J=1,NGOOD)    LEV04820
500  FORMAT(I5,E19.12,3I6)                                           LEV04830
C                                                    LEV04840
      IF(MBOUND.EQ.1) WRITE(10,510)                                  LEV04850

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510 FORMAT(/' EV = GOODEV(J) IS A GOOD EIGENVALUE OF T(1,MEV)'/ LEV04860
1' M1 = SMALLEST VALUE OF M SUCH THAT T(1,M) HAS AT LEAST'/ LEV04870
1' ONE EIGENVALUE IN THE INTERVAL (EV-TOLN, EV+TOLN)'/ LEV04880
1' TOLN(J) = DMAX1(GOODEV(J)*RELTOL, SCALEO*MULTOL)'/ LEV04890
1' M2 = SMALLEST M (IF ANY) SUCH THAT IN THE ABOVE INTERVAL'/ LEV04900
1' T(1,M) HAS AT LEAST TWO EIGENVALUES '/ LEV04910
1' IABS(MA(J)) = APPROPRIATE SIZE T-MATRIX FOR GOODEV(J)'/ LEV04920
1' INITIAL VALUE OF MA(J) IS CHOSEN HEURISTICALLY'/ LEV04930
1' PROGRAM LOOPS ON SIZE OF T-MATRIX TO GET BETTER SIZE'/ LEV04940
1' END OF SIZES OF T-MATRICES FILE 10'///) LEV04950
C LEV04960
C TERMINATE AFTER COMPUTING 1ST GUESSES AT SIZES OF THE LEV04970
C T-MATRICES REQUIRED FOR THE GIVEN EIGENVALUES? LEV04980
IF(MBOUND.EQ.1) GO TO 1390 LEV04990
C LEV05000
C IS THERE ROOM FOR ALL OF THE REQUESTED T-EIGENVECTORS? LEV05010
MTOL = 0 LEV05020
DO 520 J = 1,NGOOD LEV05030
IF(MP(J).EQ.MPMIN) GO TO 520 LEV05040
MTOL = MTOL + IABS(MA(J)) LEV05050
520 CONTINUE LEV05060
MTOL = (5*MTOL)/4 LEV05070
IF(MTOL.GT.MDIMTV.AND.NTVCON.EQ.0) GO TO 1410 LEV05080
C LEV05090
C-----LEV05100
C GENERATE A RANDOM VECTOR TO BE USED REPEATEDLY BY LEV05110
C SUBROUTINE INVERM LEV05120
C LEV05130
CALL GENRAN(RHSEED,G,KMAX) LEV05140
C LEV05150
C-----LEV05160
C LEV05170
C LOOP ON GIVEN EIGENVALUES TO COMPUTE THE CORRESPONDING LEV05180
C T-EIGENVECTOR. LEV05190
C LEV05200
MTOL = 0 LEV05210
NTVEC = 0 LEV05220
ILBIS = 0 LEV05230
DO 710 J = 1,NGOOD LEV05240
ICOUNT = 0 LEV05250
ERRMIN = 10.DO LEV05260
MABEST = MPMIN LEV05270
IF(MP(J).EQ.MPMIN) GO TO 710 LEV05280
TFLAG = 0 LEV05290
EVAL = GOODEV(J) LEV05300
TEMP = DABS(EVAL)*RELTOL LEV05310
UB = EVAL + DMAX1(STUTOL,TEMP) LEV05320
LB = EVAL - DMAX1(STUTOL,TEMP) LEV05330
530 KMAXU = IABS(MA(J)) LEV05340
C LEV05350
C SELECT A SUITABLE INCREMENT FOR THE ORDERS OF THE T-MATRICES LEV05360
C TO BE CONSIDERED IN DETERMINING APPROPRIATE SIZES FOR THE RITZ LEV05370
C VECTOR COMPUTATIONS. LEV05380
IF(ICOUNT.GT.0) GO TO 550 LEV05390
C SELECT IDELTA(J) BASED UPON THE T-MULTIPLICITY OBTAINED LEV05400

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      IF(M2(J).EQ.KMAX) GO TO 540                                LEV05410
C     M2 DETERMINED                                           LEV05420
      IDELTA(J) = ((3*M1(J) + 5*M2(J))/8 + 1 - IABS(MA(J)))/10 + 1 LEV05430
      GO TO 550                                               LEV05440
C     M2 NOT DETERMINED                                       LEV05450
540  MAMAX = MINO((11*MEV)/8 + 12, (13*M1(J))/8 + 1)         LEV05460
      IDELTA(J) = (MAMAX - IABS(MA(J)))/10 + 1               LEV05470
550  ICOUNT = ICOUNT + 1                                       LEV05480
C                                                                LEV05490
C-----LEV05500
C     TO MIMIMIZE THE EFFECT OF THE ONE-SIDED ACCEPTANCE TEST FOR LEV05510
C     EIGENVALUES IN THE BISEC SUBROUTINE, RECOMPUTE THE GIVEN LEV05520
C     EIGENVALUE AT THE SPECIFIED KMAXU                       LEV05530
C                                                                LEV05540
      CALL LBISEC(ALPHA,BETA,EPSM,EVAL,EVALN,LB,UB,TTOL,KMAXU,NEVT) LEV05550
C                                                                LEV05560
C-----LEV05570
C                                                                LEV05580
C     CHECK WHETHER OR NOT GIVEN T-MATRIX HAS AN EIGENVALUE IN THE LEV05590
C     SPECIFIED INTERVAL AND IF SO WHAT ITS T-MULTIPLICITY IS. LEV05600
C                                                                LEV05610
      IF(NEVT.EQ.1) GO TO 590                                  LEV05620
      IF(NEVT.NE.0) GO TO 570                                  LEV05630
      ILBIS = 1                                               LEV05640
      WRITE(6,560) EVAL,KMAXU                                  LEV05650
560  FORMAT('/ PROBLEM ENCOUNTERED IN RECOMPUTATION OF USER-SUPPLIED EILEV05660
1GENVALUE',E20.12/' THE SIZE T-MATRIX SPECIFIED',I6,' DOES NOT LEV05670
1HAVE AN EIGENVALUE IN THE INTERVAL SPECIFIED'/' THEREFORE NO EIGENLEV05680
1VECTOR WILL BE COMPUTED FOR THIS PARTICULAR EIGENVALUE'/) LEV05690
      GO TO 610                                               LEV05700
C                                                                LEV05710
570  IF(NEVT.GT.1) WRITE(6,580) EVAL,KMAXU                    LEV05720
580  FORMAT('/ PROBLEM ENCOUNTERED IN RECOMPUTATION OF USER-SUPPLIED LEV05730
1EIGENVALUE',E20.12/' FOR THE SIZE T-MATRIX SPECIFIED =',I6,' THE LEV05740
1GIVEN EIGENVALUE IS T-MULTIPLE IN THE INTERVAL SPECIFIED'/' SOMETHLEV05750
1ING IS WRONG, THEREFORE NO EIGENVECTOR WILL BE COMPUTED FOR THIS ELEV05760
1EIGENVALUE'/)                                             LEV05770
C                                                                LEV05780
      MP(J) = MPMIN                                           LEV05790
      MA(J) = -2*KMAXU                                         LEV05800
      GO TO 710                                               LEV05810
C                                                                LEV05820
590  CONTINUE                                               LEV05830
      ILBIS = 0                                               LEV05840
C                                                                LEV05850
      EVNEW(J) = EVALN                                         LEV05860
      EVAL = EVALN                                             LEV05870
      MTOL = MTOL+KMAXU                                        LEV05880
C                                                                LEV05890
C     IS THERE ROOM IN TVEC ARRAY FOR THE NEXT T-EIGENVECTOR? LEV05900
C     IF NOT, SKIP TO RITZ VECTOR COMPUTATIONS.              LEV05910
C     IF (MTOL.GT.MDIMTV) GO TO 720                           LEV05920
C                                                                LEV05930
      IT = 3                                                  LEV05940
      KINT = MTOL - KMAXU +1                                  LEV05950

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C                                                    LEV05960
C   RECORD THE BEGINNING AND END OF THE T-EIGENVECTOR BEING COMPUTED LEV05970
C   MINT(J) = KINT                                                    LEV05980
C   MFIN(J) = MTOL                                                    LEV05990
C                                                                    LEV06000
C-----LEV06010
C   SUBROUTINE INVERM DOES INVERSE ITERATION, I.E. SOLVES           LEV06020
C   (T(1,KMAXU) - EVAL)*U = RHS  FOR EACH EIGENVALUE TO OBTAIN THE LEV06030
C   DESIRED T-EIGENVECTOR.                                           LEV06040
C                                                                    LEV06050
C   IF(IWRITE.EQ.1) WRITE(6,600) J                                   LEV06060
600 FORMAT(/I6,'TH EIGENVALUE')                                     LEV06070
C                                                                    LEV06080
C   CALL INVERM(ALPHA,BETA,V1,TVEC(KINT),EVAL,ERROR,TERROR,EPSM,    LEV06090
1 G,KMAXU,IT,IWRITE)                                             LEV06100
C                                                                    LEV06110
C-----LEV06120
C                                                                    LEV06130
C   TERR(J) = TERROR                                                  LEV06140
C   TLAST(J) = ERROR                                                  LEV06150
C   KMAXU1 = KMAXU + 1                                                LEV06160
C   TBETA(J) = BETA(KMAXU1)*ERROR                                     LEV06170
C                                                                    LEV06180
C   AFTER EACH OF THE T-EIGENVECTORS IS COMPUTED, THE              LEV06190
C   SIZE OF THE ERROR ESTIMATE, ERROR IS CHECKED.                   LEV06200
C   IF THIS ESTIMATE IS NOT AS SMALL AS DESIRED AND                 LEV06210
C   |MA(J)| < ML(J), PROGRAM ATTEMPTS TO INCREASE THE SIZE OF |MA(J)| LEV06220
C   AND REPEAT THE T-EIGENVECTOR COMPUTATIONS.                     LEV06230
C                                                                    LEV06240
C   IF(ERROR.LT.ERTOL.OR.TFLAG.EQ.1) GO TO 700                      LEV06250
C                                                                    LEV06260
C   IF(ERROR.GE.ERRMIN) GO TO 610                                    LEV06270
C   LAST COMPONENT IS LESS THAN MINIMAL TO DATE                     LEV06280
C   ERRMIN = ERROR                                                  LEV06290
C   MABEST = MA(J)                                                  LEV06300
610 CONTINUE                                                    LEV06310
C                                                                    LEV06320
C   IF(MA(J).GT.0) ITEST = MA(J) + IDELTA(J)                        LEV06330
C   IF(MA(J).LT.0) ITEST = -(IABS(MA(J)) + IDELTA(J))               LEV06340
C   IF(IABS(ITEST).LE.ML(J).AND.ICOUNT.LE.10) GO TO 630            LEV06350
C   NEW MA(J) IS GREATER THAN MAXIMUM ALLOWED.                      LEV06360
C   IF(ERCONT.EQ.0.OR.MABEST.EQ.MPMIN) GO TO 650                   LEV06370
C   TFLAG = 1                                                        LEV06380
C   MA(J) = MABEST                                                  LEV06390
C   IF(ILBIS.EQ.0) MTOL = MTOL - KMAXU                             LEV06400
C   WRITE(6,620) MA(J)                                             LEV06410
620 FORMAT(' 10 ORDERS WERE CONSIDERED. NONE SATISFIED THE ERROR TESTLEV06420
1'/' THEREFORE USE THE BEST ORDER OBTAINED FOR THE EIGENVECTORS' LEV06430
1,I6)                                                            LEV06440
C   GO TO 530                                                       LEV06450
C                                                                    LEV06460
630 MA(J) = ITEST                                                LEV06470
C                                                                    LEV06480
C   MT = IABS(MA(J))                                               LEV06490
C   IF(IWRITE.EQ.1) WRITE(6,640) MT                                LEV06500

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640 FORMAT(/' CHANGE SIZE OF T-MATRIX TO ',I6,' RECOMPUTE T-EIGENVECTOLEV06510
1R')
C
IF(ILBIS.EQ.0) MTOL = MTOL - KMAXU
C
GO TO 530
C
C APPROPRIATE SIZE T-MATRIX WAS NOT OBTAINED
650 CONTINUE
WRITE(10,660) J,EVAL,MP(J)
660 FORMAT(/' ON 10 INCREMENTS NOT ABLE TO IDENTIFY APPROPRIATE SIZE
1T-MATRIX FOR' /
1' EIGENVALUE(',I4,') = ',E20.12,' T-MULTIPLICITY =',I4/)
IF(M2(J).EQ.KMAX) WRITE(10,670)
IF(M2(J).LT.KMAX) WRITE(10,680)
670 FORMAT(/' ORDERS TESTED RANGED FROM 5*M1(J)/4 TO APPROXIMATELY
1' /' MIN(11*MEV/8,13*M1(J)/8)') /)
680 FORMAT(/' ORDERS TESTED RANGED FROM (3*M1(J)+M2(J))/4 TO APPROXIMALEV06680
1TELY' /' (3*M1(J) + 5*M2(J))/8.') /)
WRITE(10,690)
690 FORMAT(' ALLOWING LARGER ORDERS FOR THE T-MATRICES MAY RESULT IN
1 SUCCESS' /' BUT PROBABLY WILL NOT. PROBLEM IS PROBABLY DUE TO'
1 /' LACK OF CONVERGENCE OF GIVEN EIGENVALUE, CHECK THE ERROR ESTIMLEV06730
1ATE' /)
MP(J) = MPMIN
IF(ILBIS.EQ.0) MTOL = MTOL - KMAXU
GO TO 710
700 NTVEC = NTVEC + 1
C
710 CONTINUE
NGOODC = NGOOD
GO TO 740
C
C COME HERE IF THERE IS NOT ENOUGH ROOM FOR ALL OF T-EIGENVECTORS
720 NGOODC = J-1
WRITE(6,730) J, MTOL, MDIMTV
730 FORMAT(/' NOT ENOUGH ROOM IN TVEC FOR ',I4,'TH T-VECTOR' /' T-DIMLEV06870
1ENSION REQUESTED = ',I6,' BUT TVEC HAS DIMENSION = ',I6/)
IF(NGOODC.EQ.0) GO TO 1430
MTOL = MTOL-KMAXU
C
740 CONTINUE
C
C THE LOOP ON T-EIGENVECTOR COMPUTATIONS IS COMPLETE.
C WRITE OUT THE SIZE T-MATRICES THAT WILL BE USED FOR
C THE RITZ VECTOR COMPUTATIONS.
C
WRITE(10,750)
750 FORMAT(/' SIZES OF T-MATRICES THAT WILL BE USED IN THE RITZ COMPUTLEV06990
1ATIONS'/5X,'J',16X,'GOODEV(J)',1X,'MA(J)')
C
WRITE(10,760) (J,GOODEV(J),MA(J), J=1,NGOOD)
760 FORMAT(I6,E25.14,I6)
WRITE(10,510)
C

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WRITE(6,770) MTOL LEV07060
770 FORMAT(/' THE CUMULATIVE LENGTH OF THE T-EIGENVECTORS IS',I18) LEV07070
C LEV07080
WRITE(6,780) NTVEC,NGOOD LEV07090
780 FORMAT(/I6,' T-EIGENVECTORS OUT OF',I6,' REQUESTED WERE COMPUTED') LEV07100
C LEV07110
C SAVE THE T-EIGENVECTORS ON FILE 11? LEV07120
IF(TVSTOP.NE.1.AND.SVTVEC.EQ.0) GO TO 840 LEV07130
C LEV07140
WRITE(11,790) NTVEC,MTOL,MATNO,SVSEED LEV07150
790 FORMAT(I6,3I12,' = NTVEC,MTOL,MATNO,SVSEED') LEV07160
C LEV07170
DO 820 J=1,NGOODC LEV07180
C IF MP(J) = MPMIN THEN NO SUITABLE T-EIGENVECTOR IS AVAILABLE LEV07190
C FOR THAT EIGENVALUE. LEV07200
IF(MP(J).EQ.MPMIN) WRITE(11,800) J,MA(J),GOODEV(J),MP(J) LEV07210
800 FORMAT(2I6,E20.12,I6/' TH EIGVAL,T-SIZE,EVALUE,FLAG,NO EIGVEC') LEV07220
IF(MP(J).NE.MPMIN) WRITE(11,810) J,MA(J),GOODEV(J),MP(J) LEV07230
810 FORMAT(I6,I6,E20.12,I6/' T-EIGVEC,SIZE T,EVALUE OF A,MP(J)') LEV07240
IF(MP(J).EQ.MPMIN) GO TO 820 LEV07250
KI = MINT(J) LEV07260
KF = MFIN(J) LEV07270
C LEV07280
WRITE(11,260) (TVEC(K), K=KI,KF) LEV07290
C LEV07300
820 CONTINUE LEV07310
C LEV07320
IF(TVSTOP.NE.1) GO TO 840 LEV07330
C LEV07340
WRITE(6,830) TVSTOP, NTVEC,NGOOD LEV07350
830 FORMAT(/' USER SET TVSTOP = ',I1/ LEV07360
1' THEREFORE PROGRAM TERMINATES AFTER T-EIGENVECTOR COMPUTATIONS'/ LEV07370
1' T-EIGENVECTORS THAT WERE COMPUTED ARE SAVED ON FILE 11'/ LEV07380
1I8,' T-EIGENVECTORS WERE COMPUTED OUT OF',I7,' REQUESTED'/) LEV07390
C LEV07400
GO TO 1550 LEV07410
C LEV07420
840 CONTINUE LEV07430
C IF NOT ABLE TO COMPUTE ALL THE REQUESTED T-EIGENVECTORS, LEV07440
C CONTINUE WITH THE LANCZOS VECTOR COMPUTATIONS ANYWAY? LEV07450
IF(NTVEC.NE.NGOOD.AND.LVCONT.EQ.0) GO TO 1450 LEV07460
C LEV07470
C COMPUTE THE MAXIMUM SIZE OF THE T-MATRIX USED FOR THOSE LEV07480
C EIGENVALUES WITH GOOD ERROR ESTIMATES. LEV07490
C LEV07500
KMAXU = 0 LEV07510
DO 850 J = 1,NGOODC LEV07520
MT = IABS(MA(J)) LEV07530
IF(MT.LT.KMAXU.OR.MP(J).EQ.MPMIN) GO TO 850 LEV07540
KMAXU = MT LEV07550
850 CONTINUE LEV07560
C LEV07570
IF(KMAXU.EQ.0) GO TO 1490 LEV07580
C LEV07590
WRITE(6,860) KMAXU LEV07600

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860 FORMAT(/I6,' = LARGEST SIZE T-MATRIX TO BE USED IN THE RITZ VECTORLEV07610
1 COMPUTATIONS')                                LEV07620
C                                                    LEV07630
C   COUNT THE NUMBER OF RITZ VECTORS NOT BEING COMPUTED    LEV07640
MREJEC = 0                                        LEV07650
DO 870 J=1,NGOODC                                LEV07660
870 IF(MP(J).EQ.MPMIN) MREJEC = MREJEC + 1        LEV07670
MREJET = MREJEC + (NGOOD-NGOODC)                LEV07680
IF(MREJET.NE.0) WRITE(6,880) MREJET              LEV07690
880 FORMAT('/ RITZ VECTORS ARE NOT COMPUTED FOR',I6,' OF THE EIGENVALULEV07700
1ES'/)                                           LEV07710
NACT = NGOODC - MREJEC                           LEV07720
WRITE(6,890) NGOOD,NTVEC,NACT                    LEV07730
890 FORMAT(/I6,' RITZ VECTORS WERE REQUESTED'/I6,' T-EIGENVECTORS WERELEV07740
1 COMPUTED'/I6,' RITZ VECTORS WILL BE COMPUTED'/) LEV07750
C   CHECK IF THERE ARE ANY RITZ VECTORS TO COMPUTE        LEV07760
IF(MREJEC.EQ.NGOODC) GO TO 1470                  LEV07770
C                                                    LEV07780
C   CONTINUE WITH THE LANCZOS VECTOR COMPUTATIONS?        LEV07790
IF(LVCONT.EQ.0.AND.MREJEC.NE.0) GO TO 1450      LEV07800
C                                                    LEV07810
C   NOW COMPUTE THE RITZ VECTORS. REGENERATE THE          LEV07820
C   LANCZOS VECTORS.                                       LEV07830
C                                                    LEV07840
DO 900 I = 1,NMAX                                LEV07850
900 RITVEC(I) = ZERO                              LEV07860
C                                                    LEV07870
C-----LEV07880
C   REGENERATE THE STARTING VECTOR. THIS MUST BE GENERATED AND LEV07890
C   NORMALIZED PRECISELY THE WAY IT WAS DONE IN THE EIGENVALUE LEV07900
C   COMPUTATIONS, OTHERWISE THERE WILL BE A MISMATCH BETWEEN LEV07910
C   THE T-EIGENVECTORS THAT HAVE BEEN COMPUTED FROM THE T-MATRICES LEV07920
C   READ IN FROM FILE 2 AND THE LANCZOS VECTORS THAT ARE    LEV07930
C   BEING REGENERATED.                                       LEV07940
C                                                    LEV07950
IIL = SVSEED                                     LEV07960
CALL GENRAN(IIL,G,N)                             LEV07970
C                                                    LEV07980
C-----LEV07990
C                                                    LEV08000
DO 910 J = 1,N                                   LEV08010
910 V2(J) = G(J)                                   LEV08020
C                                                    LEV08030
SUM = FINPRO(N,V2(1),1,V2(1),1)                 LEV08040
SUM = ONE/DSQRT(SUM)                             LEV08050
C                                                    LEV08060
DO 920 J = 1,N                                   LEV08070
V1(J) = ZERO                                     LEV08080
920 V2(J) = V2(J)*SUM                             LEV08090
C                                                    LEV08100
C   LOOP FOR GENERATING RITZ VECTORS (IVEC = 1,KMAXU)     LEV08110
IVEC = 1                                         LEV08120
BATA = ZERO                                       LEV08130
C                                                    LEV08140
GO TO 980                                         LEV08150

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C                                                    LEV08160
  930 CONTINUE                                       LEV08170
C                                                    LEV08180
C    COMPUTE V1 = A*V2 - BATA*V1                   LEV08190
C                                                    LEV08200
C-----LEV08210
C                                                    LEV08220
C    CALL CMATV(V2,V1,BATA)                         LEV08230
C                                                    LEV08240
C-----LEV08250
C                                                    LEV08260
C    ALFA = FINPRO(N,V1(1),1,V2(1),1)              LEV08270
C                                                    LEV08280
C    DO 940 J = 1,N                                 LEV08290
940 V1(J) = V1(J)-ALFA*V2(J)                       LEV08300
C                                                    LEV08310
C    BATA = FINPRO(N,V1(1),1,V1(1),1)              LEV08320
C    BATA = DSQRT(BATA)                            LEV08330
C    SUM = ONE/BATA                                 LEV08340
C                                                    LEV08350
C    TEMP = BETA(IVEC)                              LEV08360
C    TEMP = DABS(BATA - TEMP)/TEMP                 LEV08370
C    IF (TEMP.LT.1.0D-10)GO TO 960                 LEV08380
C                                                    LEV08390
C    THE BETA BEING REGENERATED DO NOT MATCH THE BETA IN FILE 2. LEV08400
C    SOMETHING IS WRONG IN THE LANCZOS VECTOR GENERATION. LEV08410
C    PROGRAM TERMINATES FOR USER TO CORRECT THE PROBLEM LEV08420
C    WHICH MUST BE IN THE STARTING VECTOR GENERATION OR IN LEV08430
C    THE MATRIX-VECTOR MULTIPLY SUBROUTINE CMATV SUPPLIED. LEV08440
C    THIS SUBROUTINE MUST BE THE SAME ONE USED IN THE LEV08450
C    EIGENVALUE COMPUTATIONS OR A MISMATCH WILL ENSUE. LEV08460
C                                                    LEV08470
C    WRITE(6,950) IVEC,BATA,BETA(IVEC),TEMP        LEV08480
950 FORMAT(/2X,'IVEC',16X,'BATA',10X,'BETA(IVEC)',14X,'RELDIF'/I6, LEV08490
13E20.12/' IN LANCZOS VECTOR REGENERATION THE ENTRIES OF THE TRIDIALEV08500
1GONAL MATRICES BEING'/' GENERATED ARE NOT THE SAME AS THOSE IN THELEV08510
1 MATRIX SUPPLIED ON FILE 2.'/' THEREFORE SOMETHING IS BEING INITIALEV08520
1LIZED OR COMPUTED DIFFERENTLY FROM THE WAY'/' IT WAS COMPUTED IN TLEV08530
1HE EIGENVALUE COMPUTATIONS'/' THE PROGRAM TERMINATES FOR THE USER LEV08540
1TO DETERMINE WHAT THE PROBLEM IS'//)             LEV08550
GO TO 1550                                         LEV08560
C                                                    LEV08570
C                                                    LEV08580
960 CONTINUE                                       LEV08590
C    DO 970 J = 1,N                                 LEV08600
C    TEMP = SUM*V1(J)                               LEV08610
C    V1(J) = V2(J)                                  LEV08620
970 V2(J) = TEMP                                   LEV08630
C                                                    LEV08640
980 CONTINUE                                       LEV08650
C                                                    LEV08660
C    LFIN = 0                                       LEV08670
C    DO 1000 J = 1,NGOODC                           LEV08680
C    LL = LFIN                                       LEV08690
C    LFIN = LFIN + N                                 LEV08700

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C-----LEVO9260
C                                          LEVO9270
C      CALL CMATV(RITVEC(LINT),V2,EVAL)      LEVO9280
C                                          LEVO9290
C-----LEVO9300
C                                          LEVO9310
C      COMPUTE ERROR IN RITZ VECTOR CONSIDERED AS A EIGENVECTOR OF A.  LEVO9320
C      V2 = A*RITVEC - EVAL*RITVEC          LEVO9330
C                                          LEVO9340
C      SUM = FINPRO(N,V2(1),1,V2(1),1)     LEVO9350
C      SUM = DSQRT(SUM)                     LEVO9360
C      ERR(J) = SUM                          LEVO9370
C      GAP = ABS(AMINGP(J))                  LEVO9380
C      ERRDGP(J) = SUM/GAP                  LEVO9390
C                                          LEVO9400
C      1050 CONTINUE                         LEVO9410
C                                          LEVO9420
C                                          LEVO9430
C      RITZVECTORS ARE NORMALIZED AND ERROR ESTIMATES ARE IN ERR ARRAY LEVO9440
C      AND IN ERRDGP ARRAY. STORE EVERYTHING LEVO9450
C                                          LEVO9460
C                                          LEVO9470
C      WRITE(9,1060)                         LEVO9480
C      1060 FORMAT(3X,'A-EIGENVALUE',2X,'MA(J)',3X,'A-MINGAP',6X,'AERROR',2X, LEVO9490
C      1 'AERROR/GAP',6X,'TERROR')          LEVO9500
C                                          LEVO9510
C      WRITE(13,1070)                        LEVO9520
C      1070 FORMAT(16X,'GOODEV(J)',5X,'RITZNORM',6X,'AMINGAP',5X, LEVO9530
C      1 'TBETA(J)',5X,'TLAST(J)')         LEVO9540
C                                          LEVO9550
C      DO 1100 J=1,NGOODC                    LEVO9560
C                                          LEVO9570
C      IF(MP(J).EQ.MPMIN) GO TO 1100        LEVO9580
C                                          LEVO9590
C      WRITE(9,1080)EVNEW(J),MA(J),AMINGP(J),ERR(J),ERRDGP(J),TERR(J) LEVO9600
C      1080 FORMAT(E15.8,I6,4E12.4)        LEVO9610
C                                          LEVO9620
C      WRITE(13,1090) EVNEW(J),RNORM(J),AMINGP(J),TBETA(J),TLAST(J) LEVO9630
C      1090 FORMAT(E25.14,4E13.5)         LEVO9640
C                                          LEVO9650
C      1100 CONTINUE                         LEVO9660
C                                          LEVO9670
C      IF(MREJEC.EQ.0) GO TO 1180           LEVO9680
C      WRITE(9,1110)                         LEVO9690
C      1110 FORMAT(/' RITZ VECTORS WERE NOT COMPUTED FOR THE FOLLOWING EIGENVALEVO9700
C      1LUES'/' EITHER BECAUSE THEY HAD NOT CONVERGED OR BECAUSE THE ERRORLEVO9710
C      1 ESTIMATE'/' WAS NOT AS SMALL AS DESIRED'/' ) LEVO9720
C                                          LEVO9730
C      DO 1170 J = 1,NGOODC                  LEVO9740
C      IF(MP(J).NE.MPMIN) GO TO 1170        LEVO9750
C      WRITE OUT MESSAGE FOR EACH EIGENVALUE FOR WHICH NO EIGENVECTOR LEVO9760
C      WAS COMPUTED.                        LEVO9770
C                                          LEVO9780
C      WRITE(9,1120)                         LEVO9790
C      1120 FORMAT(6X,'GOODEV(J)',3X,'MA(J)',5X,'AMINGP(J)',6X,'TLAST(J)',3X, LEVO9800

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1'MP(J)')
WRITE(9,1130) GOODEV(J),MA(J),AMINGP(J),TBETA(J),MP(J)
1130 FORMAT(E15.8,I8,2E14.4,I8)
C
WRITE(13,1140)
1140 FORMAT(/' RITZ VECTORS WERE NOT COMPUTED FOR THE FOLLOWING EIGENVALE
1LUES'/' BECAUSE THEY HAD NOT CONVERGED'/)
C
WRITE(13,1150)
1150 FORMAT(6X,'GOODEV(J)',3X,'MA(J)',3X,'M1(J)',3X,'M2(J)',3X,'MP(J)'
1/)
WRITE(13,1160) GOODEV(J),MA(J),M1(J),M2(J),MP(J)
1160 FORMAT(E15.8,4I8)
C
1170 CONTINUE
1180 CONTINUE
C
WRITE(9,1190)
1190 FORMAT(/' ABOVE ARE ERROR ESTIMATES FOR THE A AND T EIGENVECTORS'
1 ' ASSOCIATED WITH THE GOODEV LISTED IN COLUMN 1'/'
1 ' AERROR = NORM(A*X - EV*X)  TERROR = NORM(T*Y - EV*Y) '/'
1 ' WHERE T = T(1,MA(J))  X = RITZ VECTOR = V*Y  V = SUCCESSIVE'/'
1 ' LANCZOS VECTORS. AMINGAP = GAP TO NEAREST A-EIGENVALUE'//)
C
WRITE(13,1200)
1200 FORMAT(/' ABOVE ARE ERROR ESTIMATES ASSOCIATED WITH THE GOODEV'/'
1 ' RITZNORM = NORM(COMPUTED RITZ VECTOR) '/'
1 ' TBETA(J) = BETA(MA(J)+1)*Y(MA(J)),  T*Y = EVAL*Y'/'
1 ' TLAST(J) = Y(MA(J))'/'
1 ' AMINGAP = GAP TO NEAREST A-EIGENVALUE'//)
C
C NUMBER OF RITZ VECTORS COMPUTED
NCOMPU = NGOODC - MREJEC
WRITE(12,1210) N,NCOMPU,NGOODC,MATNO
1210 FORMAT(3I6,I12,' SIZE A, NO.RITZVECS, NO.EVALUES,MATNO')
C
LFIN = 0
DO 1270 J = 1,NGOODC
LINT = LFIN + 1
LFIN = LFIN + N
C
IF(MP(J).EQ.MPMIN) GO TO 1250
C RITZ VECTOR WAS COMPUTED
WRITE(12,1220) J, GOODEV(J), MP(J)
1220 FORMAT(I6,4X,E20.12,I6,' J, EIGENVAL, MP(J)')
C
WRITE(12,1230) ERR(J),ERRDGP(J)
1230 FORMAT(2E15.5,' = NORM(A*Z-EVAL*Z) AND  NORM(A*Z-EVAL*Z)/MINGAP')
C
WRITE(12,1240) (RITVEC(LL), LL=LINT,LFIN)
1240 FORMAT(4E20.12)
GO TO 1270
C NO RITZ VECTOR WAS COMPUTED FOR THIS EIGENVALUE
1250 WRITE(12,1260) J,GOODEV(J),MP(J)
1260 FORMAT(I6,4X,E20.12,I6,' J,EIGVALUE,NO RITZ VECTOR COMPUTED')

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C                                                    LEV10360
1270 CONTINUE                                       LEV10370
C                                                    LEV10380
C    DID ANY T-MATRICES INCLUDE OFF-DIAGONAL ENTRIES SMALLER THAN   LEV10390
C    DESIRED, AS SPECIFIED BY BTOL?                               LEV10400
C                                                    LEV10410
C    IF(IB.GT.0) GO TO 1300                                       LEV10420
C                                                    LEV10430
C    WRITE(6,1280) KMAXU                                         LEV10440
1280 FORMAT(/' FOR LARGEST T-MATRIX CONSIDERED',I7,' CHECK THE SIZE OF  LEV10450
1BETAS')                                           LEV10460
C                                                    LEV10470
C-----LEV10480
C                                                    LEV10490
C    CALL TNORM(ALPHA,BETA,BKMIN,TEMP,KMAXU,IBMT)                 LEV10500
C                                                    LEV10510
C-----LEV10520
C                                                    LEV10530
C    IF(IBMT.LT.0) WRITE (6,1290)                               LEV10540
1290 FORMAT(/' WARNING THE T-MATRICES FOR ONE OR MORE OF THE EIGENVALUE  LEV10550
1S CONSIDERED'/' HAD AN OFF-DIAGONAL ENTRY THAT WAS SMALLER THAN TH  LEV10560
1E BETA TOLERANCE THAT WAS SPECIFIED'/)          LEV10570
1300 CONTINUE                                       LEV10580
C                                                    LEV10590
C    GO TO 1550                                                  LEV10600
C                                                    LEV10610
1310 WRITE(6,1320) NGOOD,NMAX,MDIMRV              LEV10620
1320 FORMAT(/I4,' RITZ VECTORS WERE REQUESTED BUT THE REQUIRED DIMENSIO  LEV10630
1N',I6/' IS LARGER THAN THE USER-SPECIFIED DIMENSION OF RITVEC',I6  LEV10640
1/' THEREFORE, THE EIGENVECTOR PROCEDURE TERMINATES FOR THE USER TO  LEV10650
1 INTERVENE')                                       LEV10660
C                                                    LEV10670
C    GO TO 1550                                                  LEV10680
C                                                    LEV10690
1330 WRITE(6,1340) NOLD,N,MATOLD,MATNO           LEV10700
1340 FORMAT(/' PARAMETERS READ FROM FILE 3 DO NOT AGREE WITH THOSE SPE  LEV10710
1CIFIED BY THE USER'/' N,NOLD,MATOLD,MATNO = ',2I6,2I12/' PROGRAM T  LEV10720
1ERMINATES FOR USER TO RESOLVE PROBLEM'/)        LEV10730
C                                                    LEV10740
C    GO TO 1550                                                  LEV10750
C                                                    LEV10760
1350 WRITE(6,1360)                               LEV10770
1360 FORMAT(/' PARAMETERS IN THE ALPHA,BETA FILE HEADER DO NOT AGREE W  LEV10780
11TH PARAMTERS'/' SPECIFIED BY THE USER. THEREFORE THE PROGRAM TER  LEV10790
1MINATES FOR THE USER'/' TO RESOLVE THE PROBLEM'/) LEV10800
C                                                    LEV10810
C    GO TO 1550                                                  LEV10820
C                                                    LEV10830
1370 WRITE(6,1380) KMAX,MEV                       LEV10840
1380 FORMAT(/' ALPHA,BETA FILE HEADER GIVES KMAX =',I6/          LEV10850
1' BUT EIGENVALUES WERE COMPUTED AT MEV = ',I6,' PROGRAM STOPS'/)  LEV10860
C                                                    LEV10870
C    GO TO 1550                                                  LEV10880
C                                                    LEV10890
1390 WRITE(6,1400)                                       LEV10900

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DOUBLE PRECISION ALPHA(1),BETA(1),V1(1),V2(1),SUM,TEMP,ONE,ZERO LEM00450
REAL G(1) LEM00460
DOUBLE PRECISION FINPRO, DSQRT LEM00470
EXTERNAL MATVEC LEM00480
C-----LEM00490
C LEM00500
ZERO = 0.DO LEM00510
ONE = 1.DO LEM00520
C LEM00530
IF(MOLD1.GT.1)GO TO 30 LEM00540
C LEM00550
ALPHA/BETA GENERATION STARTS AT I = 1 LEM00560
C MOLD1 = 1 SET V1 = 0. AND V2 = RANDOM UNIT VECTOR LEM00570
C BETA(1) = ZERO LEM00580
IIL=IIX LEM00590
C LEM00600
C-----LEM00610
CALL GENRAN(IIL,G,N) LEM00620
C-----LEM00630
C LEM00640
DO 10 I = 1,N LEM00650
10 V2(I) = G(I) LEM00660
C LEM00670
C-----LEM00680
SUM = FINPRO(N,V2(1),1,V2(1),1) LEM00690
C-----LEM00700
C LEM00710
SUM = ONE/DSQRT(SUM) LEM00720
DO 20 I = 1,N LEM00730
V1(I) = ZERO LEM00740
20 V2(I) = V2(I)*SUM LEM00750
C LEM00760
C ALPHA BETA GENERATION LOOP LEM00770
30 CONTINUE LEM00780
C LEM00790
DO 60 I=MOLD1,KMAX LEM00800
SUM = BETA(I) LEM00810
C MATVEC(V2,V1,SUM) CALCULATES V1 = A*V2 - SUM*V1 LEM00820
C LEM00830
C-----LEM00840
CALL MATVEC(V2,V1,SUM) LEM00850
C-----LEM00860
C LEM00870
C-----LEM00880
SUM = FINPRO(N,V1(1),1,V2(1),1) LEM00890
C-----LEM00900
C LEM00910
ALPHA(I) = SUM LEM00920
DO 40 J=1,N LEM00930
40 V1(J) = V1(J)-SUM*V2(J) LEM00940
C LEM00950
C-----LEM00960
SUM = FINPRO(N,V1(1),1,V1(1),1) LEM00970
C-----LEM00980
C LEM00990

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WRITE(6,30) LEM01550
30 FORMAT(' PROGRAM TERMINATES BECAUSE EITHER ORDERS OF OR LABELS FOR LEM01560
1 MATRIX DISAGREE') LEM01570
GO TO 70 LEM01580
C LEM01590
40 CONTINUE LEM01600
C LEM01610
C NUMBER OF NONZERO SUBDIAGONAL ENTRIES IN EACH COLUMN IS READ LEM01620
C THEN THE CORRESPONDING ROW INDEX FOR EACH SUCH ENTRY IS READ LEM01630
READ(8,50) (ICOL(K), K=1,NZL) LEM01640
READ(8,50) (IROW(K), K=1,NZS) LEM01650
50 FORMAT(13I6) LEM01660
C LEM01670
C DIAGONAL IS READ FIRST, THEN NONZERO BELOW DIAGONAL ENTRIES LEM01680
READ(8,60) (AD(K), K=1,N) LEM01690
READ(8,60) (A(K), K=1,NZS) LEM01700
60 FORMAT(4E19.10) LEM01710
C LEM01720
C-----LEM01730
C PASS STORAGE LOCATIONS OF ARRAYS THAT DEFINE THE MATRIX TO LEM01740
C THE MATRIX-VECTOR MULTIPLY SUBROUTINE CMATV LEM01750
C LEM01760
CALL CMATVE(A,AD,ICOL,IROW,N,NZL) LEM01770
C LEM01780
C-----LEM01790
C LEM01800
RETURN LEM01810
70 STOP LEM01820
C-----END OF USPEC-----LEM01830
END LEM01840
C LEM01850
C-----MATRIX-VECTOR MULTIPLY FOR REAL SPARSE SYMMETRIC MATRICES-----LEM01860
C LEM01870
C SUBROUTINE CMATV(W,U,SUM) LEM01880
C SUBROUTINE GCMATV(W,U,SUM) LEM01890
C LEM01900
C-----LEM01910
DOUBLE PRECISION U(1),W(1),A(1),AD(1),SUM LEM01920
INTEGER IROW(1),ICOL(1) LEM01930
C-----LEM01940
C SPARSE MATRIX-VECTOR MULTIPLY FOR LANCZS U = A*W - SUM*U LEM01950
C SEE USPEC SUBROUTINE FOR DESCRIPTION OF THE ARRAYS THAT DEFINE LEM01960
C THE MATRIX LEM01970
C-----LEM01980
C LEM01990
GO TO 3 LEM02000
C STORAGE LOCATIONS OF ARRAYS ARE PASSED TO CMATV FROM USPEC LEM02010
ENTRY CMATVE(A,AD,ICOL,IROW,N,NZL) LEM02020
GO TO 4 LEM02030
C-----LEM02040
C COMPUTE THE DIAGONAL TERMS LEM02050
3 DO 10 I = 1,N LEM02060
10 U(I) = AD(I)*W(I)-SUM*U(I) LEM02070
C LEM02080
C COMPUTE BY COLUMN LEM02090

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      LLAST = 0
      DO 30 J = 1,NZL
C
      IF (ICOL(J).EQ.0) GO TO 30
      LFIRST = LLAST + 1
      LLAST = LLAST + ICOL(J)
C
      DO 20 L = LFIRST,LLAST
      I = IROW(L)
C
      U(I) = U(I) + A(L)*W(J)
      U(J) = U(J) + A(L)*W(I)
C
20 CONTINUE
C
30 CONTINUE
C
  4 RETURN
C
C-----END OF CMATV-----
      END
C
C-----MATRIX-VECTOR MULTIPLY FOR DIAGONAL TEST MATRICES-----
C
C      SUBROUTINE CMATV(W,U,SUM)
C      SUBROUTINE DCMATV(W,U,SUM)
C
C      CMATV COMPUTES U = (DIAGONAL MATRIX) * W - SUM * U
C-----
      DOUBLE PRECISION W(1),U(1),SUM
      DOUBLE PRECISION D(1)
C-----
      GO TO 3
      ENTRY MVDIAE(D,N)
      GO TO 4
C-----
C
  3 DO 10 I=1,N
  10 U(I)= D(I)*W(I) - SUM*U(I)
  4 RETURN
C
C-----END OF DIAGONAL TEST MATRIX MULTIPLY-----
      END
C
C
C-----START OF USPEC FOR DIAGONAL TEST MATRIX-----
C
C      SUBROUTINE USPEC(N,MATNO)
C      SUBROUTINE DUSPEC(N,MATNO)
C
C-----
      DOUBLE PRECISION D(1000), SHIFT, SPACE
      DOUBLE PRECISION DABS, DFLOAT
      REAL EXPLAN(20)
C-----

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C-----LEMO3200
      DOUBLE PRECISION  C0,C1,C2,HALF,ONE          LEMO3210
      REAL  EXPLAN(20)                             LEMO3220
C-----LEMO3230
      HALF = 0.5D0                                  LEMO3240
      ONE  = 1.0D0                                  LEMO3250
C-----LEMO3260
C      READ USER-SPECIFIED PARAMETERS FROM INPUT FILE 8 (FREE FORMAT)  LEMO3270
C-----LEMO3280
      READ(8,10) EXPLAN                             LEMO3290
      WRITE(6,10) EXPLAN                            LEMO3300
10  FORMAT(20A4)                                    LEMO3310
C-----LEMO3320
      READ(8,10) EXPLAN                              LEMO3330
      READ(8,*) KX,KY,C0                            LEMO3340
      N = KX*KY                                     LEMO3350
      C1 = HALF-C0                                  LEMO3360
      C2 = ONE                                       LEMO3370
C-----LEMO3380
      WRITE(6,20) N,KX,KY,C2,C0,C1                 LEMO3390
20  FORMAT(/5X,'N',4X,'KX',4X,'KY',7X,'DIAGONAL',3X,'X-CODIAGONAL',
1   3X,'Y-CODIAGONAL'/3I6,3E15.8/)                LEMO3400
C-----LEMO3420
C-----LEMO3430
      CALL PMATVE(C0,C1,C2,KX,KY)                   LEMO3440
      CALL EXEVE(C0,C1,C2,KX,KY)                    LEMO3450
      CALL EXERRP(C0,C1,C2,KX,KY)                   LEMO3460
C-----LEMO3470
      CALL EXVECP(C0,C1,C2,KX,KY)                   LEMO3470
C-----LEMO3480
C-----LEMO3490
      RETURN                                         LEMO3500
C-----LEMO3510
      END OF USPEC-----LEMO3510
      END                                           LEMO3520
C-----LEMO3530
C-----LEMO3540
      START OF CMATV-----LEMO3540
C-----LEMO3550
      CALCULATE U = A*W - SUM*U FOR REAL POISSON MATRICES  LEMO3550
C-----LEMO3560
      SUBROUTINE CMATV(W,U,SUM)                      LEMO3570
C-----LEMO3580
      SUBROUTINE PMATV(W,U,SUM)                      LEMO3580
C-----LEMO3590
C-----LEMO3600
      DOUBLE PRECISION  U(1),W(1)                   LEMO3610
      DOUBLE PRECISION  C0,C1,C2,CC0,CC1,SUM        LEMO3620
C-----LEMO3630
      GO TO 3                                         LEMO3640
      ENTRY  PMATVE(CC0,CC1,C2,KX,KY)                LEMO3650
C-----LEMO3660
C-----LEMO3670
      C0 = -CC0                                      LEMO3680
      C1 = -CC1                                      LEMO3690
      GO TO 4                                         LEMO3700
C-----LEMO3710
C-----LEMO3720
3  N = KX*KY                                         LEMO3720
      KX1 = KX-1                                     LEMO3730
      KY1 = KY-1                                     LEMO3740

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C                                                    LEM03750
  KK = 1                                                    LEM03760
  U(KK) = (C2*W(KK)+C0*W(KK+1)+C1*W(KK+KX)) - SUM*U(KK)  LEM03770
  KK = KX                                                    LEM03780
  U(KK) = (C2*W(KK)+C0*W(KK-1)+C1*W(KK+KX)) - SUM*U(KK)  LEM03790
  KK = N - KX + 1                                           LEM03800
  U(KK) = (C2*W(KK)+C0*W(KK+1)+C1*W(KK-KX)) - SUM*U(KK)  LEM03810
  KK = N                                                    LEM03820
  U(KK) = (C2*W(KK)+C0*W(KK-1)+C1*W(KK-KX)) - SUM*U(KK)  LEM03830
C                                                    LEM03840
  DO 10 J = 2,KX1                                           LEM03850
  KK = J                                                    LEM03860
  U(KK) = (C2*W(KK)+C0*W(KK-1)+C0*W(KK+1)+C1*W(KK+KX)) - SUM*U(KK) LEM03870
  KK = J+N-KX                                               LEM03880
  U(KK) = (C2*W(KK)+C0*W(KK-1)+C0*W(KK+1)+C1*W(KK-KX))-SUM*U(KK) LEM03890
10 CONTINUE                                                LEM03900
C                                                    LEM03910
  DO 30 J = 2,KY1                                           LEM03920
  KK = (J-1)*KX + 1                                         LEM03930
  U(KK) = (C2*W(KK)+C0*W(KK+1)+C1*W(KK-KX)+C1*W(KK+KX)) - SUM*U(KK) LEM03940
  DO 20 I = 2,KX1                                           LEM03950
  KK = KK + 1                                               LEM03960
  U(KK) = (C2*W(KK)+C0*W(KK-1)+C0*W(KK+1)+C1*W(KK-KX)
1 +C1*W(KK+KX)) - SUM*U(KK)                                LEM03970
20 CONTINUE                                                LEM03990
  KK = KK + 1                                               LEM04000
  U(KK) = (C2*W(KK)+C0*W(KK-1)+C1*W(KK-KX)+C1*W(KK+KX)) - SUM*U(KK) LEM04010
30 CONTINUE                                                LEM04020
C                                                    LEM04030
  4 RETURN                                                  LEM04040
C                                                    LEM04050
C-----END OF CMATV-----LEMM04060
  END                                                       LEM04070
C                                                    LEM04080
C-----START OF EXEVG-----LEMM04090
C                                                    LEM04100
C  COMPUTES TRUE EIGENVALUES OF POISSON MATRIX, GAPS BETWEEN LEM04110
C  TRUE EIGENVALUES, AND MULTIPLICITIES OF TRUE EIGENVALUES LEM04120
C  AND STORE THESE VALUES, RESPECTIVELY, IN U, G, AND MP.  LEM04130
C  THESE QUANTITIES ARE WRITTEN OUT TO FILE 9                LEM04140
C                                                    LEM04150
C  SUBROUTINE EXEVG(U,G,MP)                                   LEM04160
C                                                    LEM04170
C-----LEMM04180
  DOUBLE PRECISION  U(*)                                     LEM04190
  DOUBLE PRECISION  MACHEP, EPSM, C0, C1, C2, T0, T1, PIK, PIL, ONE, TWO LEM04200
  DOUBLE PRECISION  ATOLN, EE                               LEM04210
  REAL G(1)                                                 LEM04220
  INTEGER MP(1)                                             LEM04230
C-----LEMM04240
  DATA MACHEP/Z34100000000000000/                          LEM04250
  EPSM = 2.0D0*MACHEP                                       LEM04260
C-----LEMM04270
  GO TO 3                                                    LEM04280
  ENTRY EXEVE(C0, C1, C2, KX, KY)                            LEM04290

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      GO TO 4
      C-----LEMO4310
      3 N = KX*KY
      ONE = 1.0D0
      TWO = 2.0D0
      TO = DARCOS(-ONE)
      T1 = DFLOAT(KX+1)
      PIK = TO/T1
      T1 = DFLOAT(KY+1)
      PIL = TO/T1
      C GENERATE TRUE EIGENVALUES
      KP = 0
      DO 20 J = 1,KY
      T1 = PIL*DFLOAT(J)
      TO = C2 - TWO*C1*DCOS(T1)
      DO 10 I = 1,KX
      KP = KP+1
      T1 = PIK*DFLOAT(I)
      10 U(KP) = TO - TWO*CO*DCOS(T1)
      20 CONTINUE
      C
      C ORDER U VECTOR BY INCREASING ALGEBRAIC SIZE
      DO 40 K = 2,N
      KM1 = K-1
      DO 30 L = 1,KM1
      JJ = K-L
      IF (U(JJ+1).GE.U(JJ)) GO TO 40
      TO = U(JJ)
      U(JJ) = U(JJ+1)
      30 U(JJ+1) = TO
      40 CONTINUE
      ATOLN = DMAX1(DABS(U(1)),DABS(U(N)))*EPSM
      C
      WRITE(9,50)
      50 FORMAT(' TRUE EIGENVALUES FOR POISSON'/)
      C
      WRITE(9,60)N,KX,KY,C2,CO,C1,ATOLN
      WRITE(6,60) N,KX,KY,C2,CO,C1,ATOLN
      60 FORMAT(1X,'A-SIZE',2X,'X-DIM',2X,'Y-DIM'/3I7/
      1 5X,'A-DIAGONAL',3X,'X-CODIAGONAL',3X,'Y-CODIAGONAL',10X,'ATOLN'/
      2 4E15.8)
      C
      C DETERMINE MULTIPLICITIES FOR TRUE EIGENVALUES
      I = 1
      IDEX = 1
      J = 1
      NEXACT = 0
      70 J = J+1
      IF (J.GT.N) GO TO 80
      EE = DABS(U(J)-U(I))
      IF (EE.GT.ATOLN) GO TO 80
      IDEX = IDEX+1
      GO TO 70
      80 NEXACT = NEXACT+1
      U(NEXACT) = U(I)

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      MP(NEXACT) = IDEX                                LEM04850
C      MP(K) = MULTIPLICITY OF KTH EIGENVALUE CLUSTER FOR A    LEM04860
      IDEX = 1                                         LEM04870
      I = J                                           LEM04880
      IF (I.GT.N) GO TO 90                             LEM04890
      GO TO 70                                         LEM04900
90    CONTINUE                                         LEM04910
C                                                     LEM04920
C      MULTIPLICITIES HAVE BEEN DETERMINED             LEM04930
C      NEXACT = NUMBER OF DISTINCT A-EIGENVALUES       LEM04940
C                                                     LEM04950
      WRITE(9,100)NEXACT                               LEM04960
      WRITE(6,100)NEXACT                               LEM04970
100  FORMAT(I6,' = NUMBER OF TRUE A-EIGENVALUES WHICH ARE DISTINCT'//) LEM04980
C                                                     LEM04990
C      MINGAP CALCULATION FOR DISTINCT A-EIGENVALUES     LEM05000
      NM1 = NEXACT - 1                                 LEM05010
      G(NEXACT) = U(NM1)-U(NEXACT)                   LEM05020
      G(1) = U(2)-U(1)                                LEM05030
C                                                     LEM05040
      DO 110 J = 2,NM1                                 LEM05050
      TO = U(J)-U(J-1)                                 LEM05060
      T1 = U(J+1)-U(J)                                LEM05070
      G(J) = T1                                        LEM05080
      IF (TO.LT.T1) G(J) = -TO                        LEM05090
110  CONTINUE                                         LEM05100
C                                                     LEM05110
C      NEXACT DISTINCT A-EIGENVALUES ARE IN U IN ASCENDING ORDER LEM05120
C      MP = MULTIPLICITIES OF THE DISTINCT EIGENVALUES OF A    LEM05130
C      G = TRUE MINIMUM GAP IN A FOR EACH OF THESE EIGENVALUES LEM05140
C      G < 0 INDICATES THE LEFT-HAND GAP WAS MINIMAL.         LEM05150
C      OUTPUT MULTIPLICITIES, DISTINCT EVS, AND MINGAPS TO FILE 9 LEM05160
C                                                     LEM05170
      WRITE(9,120)                                     LEM05180
120  FORMAT(5X,'I',1X,'AMULT',5X,'TRUE A-EIGENVALUE(I)',    LEM05190
      1 3X,'A-MINGAP(I)')                               LEM05200
C                                                     LEM05210
      WRITE(9,130)(J,MP(J),U(J),G(J), J=1,NEXACT)       LEM05220
130  FORMAT(2I6,E25.16,E14.3)                         LEM05230
C                                                     LEM05240
      WRITE(9,140)                                     LEM05250
140  FORMAT(' NEXACT DISTINCT A-EIGENVALUES ARE IN ASCENDING ORDER'//
      1 ' AMULT = MULTIPLICITIES OF THE DISTINCT EIGENVALUES OF A.'//
      2 ' A-MINGAP(I) = TRUE MINIMUM GAP IN A FOR EACH EIGENVALUE.'//
      3 ' A-MINGAP(I) LT 0 INDICATES THE LEFT-HAND GAP WAS MINIMAL.'//) LEM05290
C                                                     LEM05300
C      WE ORDER U VECTOR BY INCREASING SIZE OF THE GAPS     LEM05310
C                                                     LEM05320
      DO 150 K = 1,NEXACT                               LEM05330
150  MP(K) = K                                         LEM05340
C                                                     LEM05350
      DO 170 K = 2,NEXACT                               LEM05360
      KM1 = K-1                                        LEM05370
C                                                     LEM05380
      DO 160 L = 1,KM1                                  LEM05390

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      JJ = K - L                                LEM05400
      IF (ABS(G(JJ+1)).GE.ABS(G(JJ))) GO TO 170  LEM05410
      EE = U(JJ)                                LEM05420
      U(JJ) = U(JJ+1)                          LEM05430
      U(JJ+1) = EE                             LEM05440
      GG = G(JJ)                               LEM05450
      G(JJ) = G(JJ+1)                         LEM05460
      G(JJ+1) = GG                            LEM05470
      IEE = MP(JJ)                            LEM05480
      MP(JJ) = MP(JJ+1)                      LEM05490
160 MP(JJ+1) = IEE                          LEM05500
C                                             LEM05510
170 CONTINUE                                LEM05520
C                                             LEM05530
      WRITE(9,180)                             LEM05540
180 FORMAT(5X,'K',6X,'A-MINGAP',5X,'TRUE A-EIGENVALUE(I)',2X,'A-EVNO') LEM05550
C                                             LEM05560
      WRITE(9,190)(J,G(J),U(J),MP(J), J=1,NEXACT) LEM05570
190 FORMAT(I6,E14.3,E25.16,I8)              LEM05580
C                                             LEM05590
      WRITE(9,200)                             LEM05600
200 FORMAT(' NEXACT DISTINCT A-EIGENVALUES. GAPS IN ASCENDING ORDER'/ LEM05610
2 ' A-MINGAP(I) = TRUE MINIMUM GAP IN A FOR EACH EIGENVALUE.'/ LEM05620
3 ' A-MINGAP(I) LT 0 INDICATES THE LEFT-HAND GAP WAS MINIMAL.'/ LEM05630
3 ' A-MATRIX IS BLOCK TRIDIAGONAL AND EACH DIAGONAL BLOCK IS OF ORDLE M05640
3ER NX.'/ LEM05650
4 ' NX = NUMBER OF POINTS ON EACH X-LINE. THERE ARE NY DIAGONAL BLO M05660
4CKS.'/ LEM05670
5 ' NY = NUMBER OF POINTS ON EACH Y-LINE.'/ LEM05680
5 ' A-DIAGONAL = A(K,K)'/ LEM05690
6 ' X-CODIAGONAL = A(I,I+1)'/ LEM05700
7 ' Y-CODIAGONAL = A(I,I+NX)'/ LEM05710
8 ' ----- END OF FILE 9 TRUEEV-----'//) LEM05720
C                                             LEM05730
4 RETURN                                    LEM05740
C                                             LEM05750
C-----END OF EXEVG----- LEM05760
      END                                     LEM05770
C                                             LEM05780
C-----START OF EXERR----- LEM05790
C                                             LEM05800
C FOR GIVEN COMPUTED EIGENVALUES, V(I), I=1,2,...,NG LEM05810
C COMPUTES THE CLOSEST TRUE EIGENVALUES AND THE ERROR IN THE LEM05820
C COMPUTED EIGENVALUES, AND STORES THESE RESPECTIVELY LEM05830
C IN U(I) AND IN G(MEV+I). THESE QUANTITIES ARE WRITTEN LEM05840
C TO FILE 10. LEM05850
C                                             LEM05860
      SUBROUTINE EXERR(V,U,G,MP,MEV,NG,NEXACT,IWRITE) LEM05870
C                                             LEM05880
C----- LEM05890
      DOUBLE PRECISION U(1),V(1)              LEM05900
      DOUBLE PRECISION EV,EE,T0,T1,CO,C1,C2,PIK,PIL LEM05910
      DOUBLE PRECISION ATOLN,EPSM,MACHEP,ZERO,ONE,TWO LEM05920
      REAL G(1)                                LEM05930
      INTEGER MP(1)                            LEM05940

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      JJ = K-L                                LEM06500
      IF (U(JJ+1).GE.U(JJ)) GO TO 50          LEM06510
      TO = U(JJ)                               LEM06520
      U(JJ) = U(JJ+1)                         LEM06530
40  U(JJ+1) = TO                             LEM06540
50  CONTINUE                                  LEM06550
C                                             LEM06560
      ATOLN = DMAX1(DABS(U(1)),DABS(U(N)))*EPSM LEM06570
C                                             LEM06580
C  DETERMINE MULTIPLICITIES FOR TRUE EIGENVALUES LEM06590
      I = 1                                    LEM06600
      J = 1                                    LEM06610
      NEXACT = 0                              LEM06620
60  J = J+1                                   LEM06630
      IF (J.GT.N) GO TO 70                    LEM06640
      EE = DABS(U(J)-U(I))                    LEM06650
      IF (EE.GT.ATOLN) GO TO 70               LEM06660
      IDEX = IDEX+1                          LEM06670
      GO TO 60                                LEM06680
70  NEXACT = NEXACT+1                        LEM06690
      U(NEXACT) = U(I)                       LEM06700
      I = J                                   LEM06710
      IF (I.GT.N) GO TO 80                    LEM06720
      GO TO 60                                LEM06730
80  CONTINUE                                  LEM06740
C                                             LEM06750
C  NEXACT = NUMBER OF DISTINCT A-EIGENVALUES LEM06760
C  U CONTAINS TRUE DISTINCT A-EV ORDERED BY INCREASING SIZE LEM06770
C                                             LEM06780
      IF ( IWRITE.EQ.1) WRITE(6,90)MEV,NG,NEXACT LEM06790
90  FORMAT(/3I6,' = MEV, NG, NEXACT, POISZ CASE'/ LEM06800
      1 ' TRUE ERRORS FOR GOOD EIGENVALUES'/) LEM06810
C                                             LEM06820
C  WRITE(6,61) (K,U(K), K=1,NEXACT)          LEM06830
C 61 FORMAT(4(I5,E15.8))                     LEM06840
C                                             LEM06850
C  CALCULATION OF THE TRUE ERRORS.           LEM06860
      KL = 1                                  LEM06870
      DO 110 ITEV = 1,NG                      LEM06880
      EV = V(ITEV)                            LEM06890
      K = KL                                  LEM06900
      T1 = DABS(EV - U(KL))                   LEM06910
C                                             LEM06920
      DO 100 KP = KL,NEXACT                   LEM06930
      TO = DABS(EV - U(KP))                   LEM06940
      IF (TO.GE.T1) GO TO 100                 LEM06950
      K = KP                                  LEM06960
      T1 = TO                                 LEM06970
100 CONTINUE                                  LEM06980
C                                             LEM06990
      IF (K.EQ.KL.AND.ITEV.GT.1) T1 = -T1    LEM07000
      KL = K                                  LEM07010
      MP(ITEV) = K                            LEM07020
      G(MEV+ITEV) = T1                       LEM07030
110 CONTINUE                                  LEM07040

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C                                                                    LEM07050
C   TRUE ERRORS HAVE BEEN COMPUTED OUTPUT THEM TO FILE 10          LEM07060
C   FORM HEADER FOR ERREXACT FILE 10                                LEM07070
C   WRITE(10,120)N,KX,KY,C2,C0,C1                                   LEM07080
120  FORMAT(' POISSONZ TRUE ERROR FOR GOOD EIGENVALUES'/           LEM07090
      1 5X,'N',4X,'NX',4X,'NY'/3I6//                               LEM07100
      2 5X,'A-DIAGONAL',3X,'X-CODIAGONAL',3X,'Y-CODIAGONAL'/3E15.8//) LEM07110
C                                                                    LEM07120
C   WRITE(10,130)MEV,NG,NEXACT                                     LEM07130
130  FORMAT(/3I6,' = MEV,NG,NEXACT'/1X,'T-EV NO',1X,'A-EV NO',    LEM07140
      1 10X,'GOOD EIGENVALUE',5X,'TRUEERROR',7X,'TMINGAP')        LEM07150
C                                                                    LEM07160
C   WRITE(10,140)(I,MP(I),V(I),G(MEV+I),G(I), I=1,NG)            LEM07170
140  FORMAT(2I8,E25.16,2E14.3)                                     LEM07180
C                                                                    LEM07190
C   WRITE(10,150)                                                 LEM07200
150  FORMAT(' ABOVE ARE THE TRUE ERRORS FOR POISSON GOODEV'/      LEM07210
      1 ' IF A-EV NO LT 0 THEN GOODEV HAS MULTIPLICITY GT 1'/      LEM07220
      1 ' IF TRUE ERROR LT 0 THEN MORE THAN ONE GOODEV APPROXIMATES'/ LEM07230
      1 ' THE SAME TRUE POISSON EIGENVALUE'/                        LEM07240
      1 ' IF TMINGAP LT 0 THE MINGAP IS DUE TO SPURIOUS EIGENVALUE'//) LEM07250
C                                                                    LEM07260
C   4 RETURN                                                       LEM07270
C                                                                    LEM07280
C-----END OF EXERR-----LEMM07290
      END                                                         LEM07300
C                                                                    LEM07310
C-----START OF EXVEC-----LEMM07320
C                                                                    LEM07330
C   (JVEC = 1): FOR A GIVEN RITZ VECTOR V AND EIGENVALUE X1, COMPUTES LEM07340
C   THE CLOSEST EIGENVALUE Y1 AND CORRESPONDING TRUE EIGENVECTOR U, LEM07350
C   AND THEN CALCULATES THE NORM OF THE DIFFERENCE BETWEEN        LEM07360
C   V AND U AND THE MAXIMAL DIFFERENCE BETWEEN THE COMPONENTS.   LEM07370
C   THESE QUANTITIES ARE WRITTEN TO FILE 6.                        LEM07380
C                                                                    LEM07390
C   (JVEC = 2): COMPUTES THE PROJECTION OF EACH                    LEM07400
C   OF THE TRUE EIGENVECTORS ON THE LANCZOS STARTING VECTOR      LEM07410
C   USED BY THE LANCZS SUBROUTINE AND WRITES THEM TO FILE 12.    LEM07420
C                                                                    LEM07430
C   SUBROUTINE EXVEC(U,V,X1,Y1,G,MP,IIX,JVEC,ICOUNT)              LEM07440
C                                                                    LEM07450
C-----LEMM07460
      DOUBLE PRECISION U(*),V(1)                                  LEM07470
      DOUBLE PRECISION WI(110),WJ(110),WII(110)                 LEM07480
      DOUBLE PRECISION X1,Y1,EV,EE,WS,PIK,PIL,SUM,PROJ,TEMP,S    LEM07490
      DOUBLE PRECISION ATOLN,EPSM,MACHEP,ZERO,HALF,ONE,TWO      LEM07500
      DOUBLE PRECISION C0,C1,C2,TO,T1,T2                         LEM07510
      REAL G(1),GG                                               LEM07520
      INTEGER MP(1)                                              LEM07530
      DOUBLE PRECISION FINPRO                                     LEM07540
C-----LEMM07550
C   THIS PROGRAM CALCULATES THE TRUE EIGENVALUES AND EIGENVECTORS LEM07560
C   OF THE POISSON MATRIX A OF ORDER N = KX*KY                   LEM07570
C   A CONSISTS OF KY TRIDIAGONAL BLOCKS OF ORDER KX             LEM07580
C   KX = X-DIMENSION      KY = Y-DIMENSION.                      LEM07590

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TWO = 2.0D0                                LEM08150
TO = DARCOS(-ONE)                          LEM08160
T1 = DFLOAT(KX+1)                          LEM08170
PIK = TO/T1                                LEM08180
T2 = DFLOAT(KY+1)                          LEM08190
PIL = TO/T2                                LEM08200
WS = TWO/DSQRT(T1*T2)                      LEM08210
C                                           LEM08220
C GENERATE WI WJ VECTORS                    LEM08230
KP = 0                                      LEM08240
DO 20 J = 1,KY                              LEM08250
T1 = PIL*DFLOAT(J)                          LEM08260
WJ(J) = T1                                  LEM08270
TO = C2 - TWO*C1*DCOS(T1)                  LEM08280
DO 10 I = 1,KX                              LEM08290
KP = KP+1                                    LEM08300
T1 = PIK*DFLOAT(I)                          LEM08310
WI(I) = T1                                  LEM08320
10 U(KP) = TO - TWO*C0*DCOS(T1)            LEM08330
20 CONTINUE                                  LEM08340
C U(KP) = EV(I,J) = C2 - 2*C1*COS(PIL*J) - 2*C0*COS(PIK*I) LEM08350
C                                           LEM08360
C INITIALIZE MP VECTOR                      LEM08370
DO 30 K = 1,N                                LEM08380
30 MP(K) = K                                LEM08390
C                                           LEM08400
C WE ORDER U VECTOR BY INCREASING SIZE OF THE EVS LEM08410
DO 50 K = 2,N                                LEM08420
KM1 = K-1                                    LEM08430
C                                           LEM08440
DO 40 L = 1,KM1                              LEM08450
JJ = K - L                                  LEM08460
IF (U(JJ+1).GE.U(JJ)) GO TO 50              LEM08470
EE = U(JJ)                                  LEM08480
U(JJ) = U(JJ+1)                              LEM08490
U(JJ+1) = EE                                  LEM08500
IEE = MP(JJ)                                  LEM08510
MP(JJ) = MP(JJ+1)                            LEM08520
40 MP(JJ+1) = IEE                            LEM08530
C                                           LEM08540
50 CONTINUE                                  LEM08550
C                                           LEM08560
ATOLN = DMAX1(DABS(U(1)),DABS(U(N)))*EPSM   LEM08570
C                                           LEM08580
IF (ICOUNT.EQ.1) WRITE(6,60) N,KX,KY,JVEC,C2,C0,C1,ATOLN LEM08590
60 FORMAT(/' TRUE ERRORS FOR CONVERGED GOODEV'/ LEM08600
1 4I6,' = N KX KY JVEC'// LEM08610
1 4E12.5,' = C2 C0 C1 ATOLN'//) LEM08620
C                                           LEM08630
C KP = MP(K) MEANS EIGENVALUE U(K) CORRESPONDS TO EIGENVECTOR W(KP) LEM08640
C COMPUTE TOLERANCE USED IN COMPUTING TRUE MULTIPLICITIES LEM08650
C                                           LEM08660
IF (JVEC.EQ.1) GO TO 180                    LEM08670
C                                           LEM08680
C JVEC = 2 SO CALCULATE PROJECTIONS AND WRITE IN FILE 12 LEM08690

```

```

C                                                    LEM08700
      WRITE(12,70)                                    LEM08710
70  FORMAT(' PROJECTIONS OF LANCZOS STARTING VECTOR ON A-EIGENVECS') LEM08720
C                                                    LEM08730
      WRITE(12,80)N,KX,KY,IIX,C2,C0,C1,ATOLN         LEM08740
80  FORMAT(1X,'A-SIZE',2X,'X-DIM',2X,'Y-DIM',6X,'SVSEED'/3I7,I12/ LEM08750
      1 5X,'A-DIAGONAL',3X,'X-CODIAGONAL',3X,'Y-CODIAGONAL',5X,'ATOLN'/ LEM08760
      2 3E15.8,E10.3)                                LEM08770
C                                                    LEM08780
      WRITE(12,90)                                    LEM08790
90  FORMAT(5X,'PROJECTION',8X,'TRUE A-EIGENVALUE',1X,'EV NO' LEM08800
      1,2X,'VEC NO')                                  LEM08810
C                                                    LEM08820
C  GENERATE SAME RANDOM UNIT VECTOR USED IN THE LANCZS RECURSIONS. LEM08830
      IIL=IIX                                         LEM08840
C                                                    LEM08850
C-----LEMO8860
      CALL GENRAN(IIL,G,N)                            LEM08870
C-----LEMO8880
C                                                    LEM08890
      DO 100 I = 1,N                                  LEM08900
100  V(I) = G(I)                                       LEM08910
C                                                    LEM08920
C-----LEMO8930
      SUM = FINPRO(N,V(1),1,V(1),1)                  LEM08940
C-----LEMO8950
C                                                    LEM08960
      SUM = 1.DO/DSQRT(SUM)                           LEM08970
C                                                    LEM08980
C                                                    LEM08990
      DO 110 I = 1,N                                  LEM08990
110  V(I) = V(I)*SUM                                   LEM09000
C                                                    LEM09010
C  DETERMINE UNIT EIGENVECTOR W ASSOCIATED WITH EACH EV(I,J) = Y1 LEM09020
C  AND CALCULATE THE PROJECTION G(K) OF U ON THE STARTING VECTOR V LEM09030
C  A*U = EV*U      WS = 1/||WU||: WU = UNSCALED EIGENVECTOR LEM09040
C                                                    LEM09050
      DO 160 K =1,N                                    LEM09060
C  DETERMINE I J FROM K: MP(K) = KP = (J-1)*KX+I LEM09070
      KP = MP(K)                                       LEM09080
      I = MOD(KP,KX)                                   LEM09090
      IF (I.EQ.0) I = KX                               LEM09100
      T1 = WI(I)                                       LEM09110
      J = 1 + (KP-1)/KX                                LEM09120
      T0 = WJ(J)                                       LEM09130
      T0 = WJ(J)                                       LEM09140
C                                                    LEM09150
      Y1 = C2 - TWO*C1*DCOS(WJ(J)) - TWO*C0*DCOS(WI(I)) LEM09160
C  Y1 = EV(I,J)                                       LEM09170
C                                                    LEM09180
      DO 120 II = 1,KX                                  LEM09190
      T2 = T1*DFLOAT(II)                               LEM09200
120  WII(II) = WS*DSIN(T2)                             LEM09210
C                                                    LEM09220
      KV = 0                                           LEM09230
      DO 140 JJ = 1,KY                                  LEM09240

```

```

      T2 = T0*DFLOAT(JJ)                                LEM09250
      T2 = DSIN(T2)                                     LEM09260
C
      DO 130 II = 1,KX                                  LEM09270
      KV = KV + 1                                       LEM09280
130  U(KV) = T2*WII(II)                                 LEM09290
C
140  CONTINUE                                          LEM09300
C
C      U IS UNIT EIGENVECTOR OF A ASSOCIATED WITH EV(I,J) = Y1  LEM09310
C      G(K) IS THE PROJECTION OF U ON V FOR Y1           LEM09320
C
C-----LEMM09330
      PROJ = FINPRO(N,U(1),1,V(1),1)                   LEM09340
C-----LEMM09350
C
      TEMP = DABS(PROJ)                                 LEM09360
      G(K) = TEMP                                       LEM09370
C
C      DESIRED PROJECTION HAS BEEN COMPUTED OUTPUT IT TO FILE 12.  LEM09380
C      WRITE(12,150) G(K),Y1,K,MP(K)                   LEM09390
150  FORMAT(E15.8,E25.16,I6,I8)                         LEM09400
C
160  CONTINUE                                          LEM09410
C
      WRITE(12,170)                                     LEM09420
170  FORMAT(' ----- END OF FILE 12 PROJECT -----'//) LEM09430
C
      GO TO 310                                         LEM09440
C
C      JVEC = 1                                         LEM09450
C
C      X1 IS AN INPUT PARAMETER. WE CALCULATE TRUE      LEM09460
C      A-EIGENVALUE WHICH IS CLOSEST TO X1, LABEL IT Y1 AND CALCULATE LEM09470
C      UNIT EIGENVECTOR OF A ASSOCIATED WITH Y1. A*U = Y1*U, ||U|| = 1. LEM09480
C      Y1 = EV(I,J). EIGENVALUES OF A ARE ORDERED BY INCREASING SIZE. LEM09490
C      V = RITZ VECTOR ASSOCIATED WITH GOODEV X1       LEM09500
C
180  CONTINUE                                          LEM09510
      KX1 = 0                                           LEM09520
      IF (X1.LE.U(1)) KX1 = 1                            LEM09530
      IF (X1.GE.U(N)) KX1 = N                            LEM09540
      NM1 = N-1                                         LEM09550
      IF (KX1.NE.0) GO TO 200                            LEM09560
C
      DO 190 KVEC = 2,N                                  LEM09570
      IF (X1.GE.U(KVEC)) GO TO 190                        LEM09580
C      U(KVEC-1).LE.X1.LT.U(KVEC)                       LEM09590
      T1 = X1 - U(KVEC-1)                                LEM09600
      T2 = U(KVEC) - X1                                  LEM09610
      KX1 = KVEC - 1                                     LEM09620
      IF (T1.GT.T2) KX1 = KVEC                           LEM09630
      GO TO 200                                          LEM09640
190  CONTINUE                                          LEM09650
C
      GO TO 310                                         LEM09660

```

```

200 Y1 = U(KX1)
C
IF (KX1.EQ.1) EE = U(2) - U(1)
IF (KX1.EQ.N) EE = U(N) - U(NM1)
IF (KX1.EQ.1.OR.KX1.EQ.N) GO TO 210
EE = DMIN1(U(KX1+1)-U(KX1),U(KX1)-U(KX1-1))
210 CONTINUE
C
TO = DABS(ONE - X1/Y1)
C
WRITE(6,220) N,KX1,ICOUNT,Y1,X1,TO,EE
220 FORMAT(3I8,' = N, A-EV NUMBER,RITZ NUMBER'//
1 18X,' TRUEEV',19X,'GOODEV',4X,'RELEERROR',4X,'A-MINGAP'//
1 2E25.16,2E12.3/)
C
IF (EE.GT.ATOLN) GO TO 240
C
WRITE(6,230)
230 FORMAT(' Y1 IS A MULTIPLE EIGENVALUE OF A SO WE EXIT'/)
C
GO TO 310
C
Y1 IS TOEPLITZ EIGENVALUE CLOSEST TO X1.
C
CALCULATION OF EIGENVECTOR ASSOCIATED WITH EIGENVALUE Y1
C
A*U = Y1*U
C
DETERMINE I J FROM K: MP(K) = KP = (J-1)*KX+I
240 CONTINUE
K = KX1
KP = MP(K)
I = MOD(KP,KX)
IF (I.EQ.0) I = KX
T1 = WI(I)
J = 1 + (KP-1)/KX
T2 = WJ(J)
C
DO 250 II = 1,KX
TO = T1*DFLOAT(II)
250 WII(II) = WS*DSIN(TO)
C
KV = 0
DO 270 JJ = 1,KY
TO = T2*DFLOAT(JJ)
TO = DSIN(TO)
C
DO 260 II = 1,KX
KV = KV + 1
260 U(KV) = TO*WII(II)
C
270 CONTINUE
C
U IS UNIT TRUE EIGENVECTOR OF A ASSOCIATED WITH Y1
C
V IS UNIT RITZVECTOR OF A ASSOCIATED WITH X1
C
KK = 0
S = ONE

```

LEM09800  
LEM09810  
LEM09820  
LEM09830  
LEM09840  
LEM09850  
LEM09860  
LEM09870  
LEM09880  
LEM09890  
LEM09900  
LEM09910  
LEM09920  
LEM09930  
LEM09940  
LEM09950  
LEM09960  
LEM09970  
LEM09980  
LEM09990  
LEM10000  
LEM10010  
LEM10020  
LEM10030  
LEM10040  
LEM10050  
LEM10060  
LEM10070  
LEM10080  
LEM10090  
LEM10100  
LEM10110  
LEM10120  
LEM10130  
LEM10140  
LEM10150  
LEM10160  
LEM10170  
LEM10180  
LEM10190  
LEM10200  
LEM10210  
LEM10220  
LEM10230  
LEM10240  
LEM10250  
LEM10260  
LEM10270  
LEM10280  
LEM10290  
LEM10300  
LEM10310  
LEM10320  
LEM10330  
LEM10340

	T1 = ZERO	LEM10350
C		LEM10360
	DO 280 K = 1,N	LEM10370
	IF (DABS(U(K)).LE.T1) GO TO 280	LEM10380
	T1 = DABS(U(K))	LEM10390
	KK = K	LEM10400
280	CONTINUE	LEM10410
	IF (U(KK)*V(KK).LT.ZERO) S = - ONE	LEM10420
C		LEM10430
	KK = 0	LEM10440
	T1 = ZERO	LEM10450
	T2 = ZERO	LEM10460
	DO 290 K = 1,N	LEM10470
	TEMP = DABS(S*U(K) - V(K))	LEM10480
	T2 = T2 + TEMP**2	LEM10490
	IF (TEMP.LE.T1) GO TO 290	LEM10500
	KK = K	LEM10510
	T1 = TEMP	LEM10520
290	CONTINUE	LEM10530
C		LEM10540
	T2 = DSQRT(T2)	LEM10550
	WRITE(6,300) KK,T1,T2	LEM10560
300	FORMAT(' EIGENVECTOR ERROR. MAX ERROR AT COMPONENT = ',I6/ 1 ' MAX DABS(TRUEVEC(K)-RITZVEC(K)) = ',E12.5/ 1 ' NORM(TRUEVEC-RITZVEC) = ',E12.5/)	LEM10570
		LEM10580
		LEM10590
C		LEM10600
310	CONTINUE	LEM10610
C		LEM10620
4	RETURN	LEM10630
C		LEM10640
C-----	END OF EXVEC-----	LEM10650
	END	LEM10660

## 2.6 LESUB: Other Subroutines used by the Codes in Chapters 2, 3, 4, 5

```

C----- LES00010
C LES00020
C LESUB LES00030
C LES00040
C----- LES00050
C Authors: Jane Cullum and Ralph A. Willoughby (Deceased) LES00060
C Los Alamos National Laboratory LES00070
C Los Alamos, New Mexico 87544 LES00080
C LES00090
C E-mail: cullumj@lanl.gov LES00100
C LES00110
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C LES00210
C This header is not to be removed from these codes. LES00220
C LES00230
C REFERENCE: Cullum and Willoughby, Chapters 1,2,3,4 LES00231
C Lanczos Algorithms for Large Symmetric Eigenvalue Computations LES00232
C VOL. 1 Theory. Republished as Volume 41 in SIAM CLASSICS in LES00233
C Applied Mathematics, 2002. SIAM Publications, LES00234
C Philadelphia, PA. USA LES00235
C LES00236
C LES00237
C (1) REAL SYMMETRIC LES00240
C (2) HERMITIAN MATRICES LES00250
C (3) FACTORED INVERSES OF REAL SYMMETRIC MATRICES AND LES00260
C (4) REAL SYMMETRIC GENERALIZED,  $A*X = EVAL*B*X$  WHERE LES00270
C B IS POSITIVE DEFINITE, CHOLESKY FACTOR AVAILABLE LES00280
C LES00290
C ACCORDING TO PFORT THESE SUBROUTINES ARE PORTABLE EXCEPT FOR: LES00300
C (1) THE COMPLEX*16 VARIABLES AND THE CORRESPONDING FUNCTIONS LES00310
C FOR COMPLEX VARIABLES, DCMLPX, DREAL AND DCONJG USED IN LES00320
C THE SUBROUTINE CINPRD (USED ONLY IN CASE (2), HERMITIAN) LES00330
C (2) THE ENTRY IN THE SUBROUTINE LPERM USED TO PASS THE LES00340
C PERMUTATION FROM THE UPSEC SUBROUTINE TO LPERM. (USED LES00350
C ONLY IN CASES (3) AND (4), INVERSE AND GENERALIZED). LES00360
C LES00370
C SUBROUTINES BISEC, INVERR, TNORM, LUMP, ISOEV, PRTEST, AND LES00380
C INVERM ARE USED WITH THE LANCZOS EIGENVALUE LES00390
C PROGRAMS LEVAL, HLEVAL, LIVAL AND LGVAL. STURMI, LES00400
C INVERM, LBISEC, AND TNORM ARE USED WITH THE LES00410
C EIGENVECTOR PROGRAMS LEVEC, HLEVEC, LIVEC AND LES00420
C LGVEC. LPERM IS USED WITH LIVEC AND LGVEC. LES00430

```

```

C          IN THE HERMITIAN CASE, THE SUBROUTINE CINPRD      LES00440
C          IS ALSO USED.                                     LES00450
C                                                         LES00460
C-----COMPUTE T-EIGENVALUES BY BISECTION-----LES00470
C                                                         LES00480
C          SUBROUTINE BISEC(ALPHA,BETA,BETA2,VB,VS,LBD,UBD,EPS,TTOL,MP,
1 NINT,MEV,NDIS,IC,IWRITE)                                LES00490
C                                                         LES00500
C                                                         LES00510
C-----LES00520
C          DOUBLE PRECISION ALPHA(1),BETA(1),BETA2(1),VB(1),VS(1) LES00530
C          DOUBLE PRECISION LBD(1),UBD(1),EPS,EPT,EPO,EP1,TEMP,TTOL LES00540
C          DOUBLE PRECISION ZERO,ONE,HALF,YU,YV,LB,UB,XL,XU,X1,X0,XS,BETAM LES00550
C          INTEGER MP(1),IDEF(100)                         LES00560
C          DOUBLE PRECISION DABS, DSQRT, DMAX1, DMIN1, DFLOAT LES00570
C-----LES00580
C          COMPUTES EIGENVALUES OF T(1,MEV) BY LOOPING INTERNALLY ON THE LES00590
C          USER-SPECIFIED INTERVALS, (LB(J),UB(J)), J = 1,NINT. INTERVALS LES00600
C          ARE TREATED AS OPEN ON THE LEFT AND CLOSED ON THE RIGHT. LES00610
C          THE BISEC SUBROUTINE SIMULTANEOUSLY LABELS SPURIOUS T-EIGENVALUES LES00620
C          AND DETERMINES THE T-MULTIPLICITIES OF EACH GOOD T-EIGENVALUE. LES00630
C          SPURIOUS T-EIGENVALUES ARE LABELLED BY A T-MULTIPLICITY = 0. LES00640
C          ANY T-EIGENVALUE WITH A T-MULTIPLICITY >= 1 IS 'GOOD'. LES00650
C                                                         LES00660
C          IF IWRITE = 0 THEN MOST OF THE WRITES TO FILE 6 ARE NOT LES00670
C          ACTIVATED.                                       LES00680
C                                                         LES00690
C          NOTE THAT PROGRAM ASSUMES THAT NO MORE THAN MMAX/2 EIGENVALUES LES00700
C          OF T(1,MEV) ARE TO BE COMPUTED IN ANY ONE OF THE SUBINTERVALS LES00710
C          CONSIDERED, WHERE MMAX = DIMENSION OF VB SPECIFIED BY THE USER LES00720
C          IN THE MAIN PROGRAM LEVEL.                       LES00730
C                                                         LES00740
C          ON ENTRY                                         LES00750
C          BETA2(J) IS SET = BETA(J)*BETA(J). THE STORAGE FOR BETA2 COULD LES00760
C          BE ELIMINATED BY RECOMPUTING THE BETA(J)**2 FOR EACH STURM LES00770
C          SEQUENCE.                                        LES00780
C                                                         LES00790
C          EPS = 2*MACHEP = 4.4 * 10**-16 ON IBM 3081.     LES00800
C          TTOL = EPS*TKMAX WHERE                           LES00810
C          TKMAX = MAX(|ALPHA(K)|,BETA(K), K=1,KMAX)        LES00820
C                                                         LES00830
C          ON EXIT                                          LES00840
C          NDIS = TOTAL NUMBER OF COMPUTED DISTINCT EIGENVALUES OF LES00850
C          T(1,MEV) ON THE UNION OF THE (LB,UB) INTERVALS. LES00860
C          VS = COMPUTED DISTINCT EIGENVALUES OF T(1,MEV) IN ALGEBRAICALLY- LES00870
C          INCREASING ORDER                                LES00880
C          MP = CORRESPONDING T-MULTIPLICITIES OF THESE EIGENVALUES LES00890
C          MP(I) = (0,1,MI), MI>1, I=1,NDIS MEANS:         LES00900
C          (0) V(I) IS SPURIOUS                             LES00910
C          (1) V(I) IS ISOLATED AND GOOD                   LES00920
C          (MI) V(I) IS MULTIPLE AND HENCE A CONVERGED GOOD T-EIGENVALUE. LES00930
C          IC = TOTAL NUMBER OF STURMS USED                LES00940
C                                                         LES00950
C          DEFAULTS                                         LES00960
C          ISKIP = 0 INITIALLY. IF DEFAULT OCCURS ON J-TH SUB-INTERVAL, SET LES00970
C          ISKIP=ISKIP+1 AND IDEF(ISKIP) = J               LES00980

```





```

          ICT = 0
C
C          START OF T-EIGENVALUE CALCULATIONS
          X1 = UB
          ISTURM = 1
          GO TO 330
C          FORWARD STURM CALCULATION TO DETERMINE NA = NO. T-EIGENVALUES > UB
50 NA = NEV
C
          X1 = LB
          ISTURM = 2
          GO TO 330
C          FORWARD STURM CALC TO DETERMINE MT = NO. T-EIGENVALUES ON (LB,UB)
60 CONTINUE
          MT=NEV
          ICT = ICT +2
C
          WRITE(6,70)MT,NA
70 FORMAT(/2I6,' = NO. TMEV ON (LB,UB) AND NO. .GT. UB'/)
C
C          DEFAULT TEST: IS ESTIMATED NUMBER OF STURMS > MXSTUR?
          IEST = 30*MT
          IF (IEST.LT.MXSTUR) GO TO 90
C
          WRITE(6,80)
80 FORMAT(/' ESTIMATED NUMBER OF STURMS REQUIRED EXCEEDS USER LIMIT'
1/' SKIP THIS SUBINTERVAL')
          GO TO 110
C
90 CONTINUE
C
          IF (MT.GE.1) GO TO 120
C
          WRITE(6,100)
100 FORMAT(/' THERE ARE NO T-EIGENVALUES ON THIS INTERVAL')/)
C
110 ISKIP = ISKIP+1
          IDEF(ISKIP) = JIND
          GO TO 430
C
C          REGULAR CASE.
120 CONTINUE
C
          IF (IWRITE.NE.0) WRITE(6,130)
130 FORMAT(/' DISTINCT T-EIGENVALUES COMPUTED USING BISEC'/
1 13X,'T-EIGENVALUE',2X,'TMULT',3X,'MD',4X,'NG')
C
C          SET UP INITIAL UPPER AND LOWER BOUNDS FOR T-EIGENVALUES
          DO 140 I=1,MT
          VB(I) = LB
          MTI = MT + I
140 VB(MTI) = UB
C
C          CALCULATE T-EIGENVALUES FROM LB UP TO UB  K = MT,...,1
C          MAIN LOOP FOR FINDING KTH T-EIGENVALUE

```

```

C
    K = MT
150 CONTINUE
    ICO = 0
    XL = VB(K)
    MTK = MT+K
    XU = VB(MTK)
C
    ISTURM = 3
    X1 = XU
    ICO = ICO + 1
    GO TO 330
C    FORWARD STURM CALCULATION AT XU
160 NU=NEV
C
C    BISECTION LOOP FOR KTH T-EIGENVALUE. TEST X1=MIDPOINT OF (XL,XU)
    ISTURM = 4
170 CONTINUE
    X1 = (XL+XU)*HALF
    XS = DABS(XL)+DABS(XU)
    X0 = XU-XL
    EPT = EPS*XS+EP1
C
C    EPT IS CONVERGENCE TOLERANCE FOR KTH T-EIGENVALUE
C
    IF (X0.LE.EPT) GO TO 230
C
C    T-EIGENVALUE HAS NOT YET CONVERGED
C
    ICO = ICO + 1
    GO TO 330
C    FORWARD STURM CALCULATION AT CURRENT T-EIGENVALUE APPROXIMATION.
180 CONTINUE
C
C    UPDATE T-EIGENVALUE INTERVAL (XL,XU)
C
    IF (NEV.LT.K) GO TO 190
C
C    NUMBER OF T-EIGENVALUES NEV = K
    XL = X1
    GO TO 170
190 CONTINUE
C    NUMBER OF T-EIGENVALUES NEV<K
    XU = X1
    NU = NEV
C
C    UPDATE OF T-EIGENVALUE BOUNDS
C
    IF (NEV.EQ.0) GO TO 210
C
    DO 200 I = 1,NEV
200 VB(I) = DMAX1(X1,VB(I))
C
210 NEV1 = NEV+1
C

```

```

DO 220 II = NEV1,K                                LES02640
  I = MT+II                                       LES02650
220 VB(I) = DMIN1(X1,VB(I))                       LES02660
C                                                  LES02670
  GO TO 170                                       LES02680
C                                                  LES02690
C  END (XL,XU) BISECTION LOOP FOR KTH T-EIGENVALUE ON (LB,UB) LES02700
C  TEST FOR T-MULTIPLICITY AND IF SIMPLE THEN TEST FOR SPURIOUSNESS LES02710
C                                                  LES02720
230 CONTINUE                                       LES02730
  NDIS = NDIS+1                                   LES02740
  MD = MD+1                                       LES02750
  VS(NDIS) = X1                                   LES02760
C                                                  LES02770
  JSTURM = 1                                       LES02780
  X1 = XL-EPO                                     LES02790
  GO TO 370                                       LES02800
C  BACKWARD STURM CALCULATION                     LES02810
240 KL = KEV                                       LES02820
  JL = JEV                                       LES02830
C                                                  LES02840
  JSTURM = 2                                       LES02850
  ICO = ICO + 2                                   LES02860
  X1 = XU+EPO                                     LES02870
  GO TO 370                                       LES02880
C  BACKWARD STURM CALCULATION                     LES02890
250 JU = JEV                                       LES02900
  KU = KEV                                       LES02910
C                                                  LES02920
C  FOR T(1,MEV)                                   LES02930
C  NU - KU = NO. T-EIGENVALUES ON (XU, XU + EPO) LES02940
C  KL - KU = NO. T-EIGENVALUES ON (XL - EPO, XU + EPO) LES02950
C                                                  LES02960
C  FOR T(2,MEV)                                   LES02970
C  JL -JU = NO. T-EIGENVALUES ON (XL - EPO, XU + EPO) LES02980
C                                                  LES02990
C  IS THIS A SIMPLE T-EIGENVALUE?                LES03000
C                                                  LES03010
  IF (KL-KU-1.EQ.0) GO TO 290                     LES03020
C                                                  LES03030
C  VS(NDIS) = KTH-T-EIGENVALUE OF (LB,UB) IS MULTIPLE AND HENCE GOOD LES03040
  IF (KU.EQ.NU) GO TO 280                         LES03050
C  CONTINUE TO CHECK FOR T-MULTIPLICITY          LES03060
260 CONTINUE                                       LES03070
  ISTURM = 5                                       LES03080
  X1 = X1+EPO                                     LES03090
  ICO = ICO + 1                                   LES03100
  GO TO 330                                       LES03110
C  FORWARD STURM CALCULATION                     LES03120
270 KNE = KU-NEV                                   LES03130
  KU = NEV                                       LES03140
  IF (KNE.NE.0) GO TO 260                         LES03150
C  SPECIFY T-MULTIPLICITY = MP(NDIS)             LES03160
280 MPEV = KL-KU                                   LES03170
  KNEW = KU                                       LES03180

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DO 400 II = 1,MEV                                LES03740
  I = MP1-II                                      LES03750
  IF (YU.NE.ZERO) GO TO 380                       LES03760
  YV = BETA(I+1)/EPS                              LES03770
  GO TO 390                                        LES03780
380 YV = BETA2(I+1)/YU                            LES03790
390 YU = X1-ALPHA(I)-YV                          LES03800
  JEV = 0                                         LES03810
  IF (YU.GE.ZERO) GO TO 400                      LES03820
  KEV = KEV+1                                    LES03830
  JEV = 1                                         LES03840
400 CONTINUE                                     LES03850
  JEV = KEV-JEV                                  LES03860
C                                                 LES03870
  GO TO (240,250), JSTURM                        LES03880
C                                                 LES03890
C  KEV = -NA + (NUMBER OF T(1,MEV) EIGENVALUES) > X1 LES03900
C  JEV = -NA + (NUMBER OF T(2,MEV) EIGENVALUES) > X1 LES03910
C  SET PARAMETERS FOR NEXT INTERVAL              LES03920
410 CONTINUE                                     LES03930
  IC = ICT+IC                                    LES03940
  MXSTUR = MXSTUR-ICT                          LES03950
C                                                 LES03960
  WRITE(6,420) JIND,NG,MD                       LES03970
420 FORMAT(/' T-EIGENVALUE CALCULATION ON INTERVAL',I6,' IS COMPLETE' LES03980
  1 /3X,'NO. GOOD',3X,'NO. DISTINCT'/I10,I13)   LES03990
C                                                 LES04000
430 CONTINUE                                     LES04010
C                                                 LES04020
C  END LOOP ON THE SUBINTERVALS (LB(J),UB(J)), J=1,NINT LES04030
C  ISKIP OUTPUT                                  LES04040
C                                                 LES04050
  IF (ISKIP.GT.0) WRITE(6,440) ISKIP             LES04060
440 FORMAT(' BISEC DEFAULTED ON',I3,3X,' INTERVALS'/ LES04070
  1 ' DEFAULTS OCCUR IF AN INTERVAL HAS NO T-EIGENVALUES'/ LES04080
  2 ' OR THE STURM ESTIMATE EXCEEDS THE USER-SPECIFIED LIMIT'/) LES04090
C                                                 LES04100
  IF (ISKIP.GT.0) WRITE(6,450) (IDEF(I), I=1,ISKIP) LES04110
450 FORMAT(' BISEC DEFAULTED ON INTERVALS'/(10I8)) LES04120
C                                                 LES04130
C  RESET BETA AT I = MP1                        LES04140
C  BETA(MP1) = BETAM                           LES04150
C-----END OF BISEC-----LES04160
  RETURN                                        LES04170
  END                                          LES04180
C                                                 LES04190
C-----INVERSE ITERATION ON T(1,MEV)-----LES04200
C                                                 LES04210
  SUBROUTINE INVERR(ALPHA,BETA,V1,V2,VS,EPS,G,MP,MEV,MMB,NDIS,NISO, LES04220
  1 N,IKL,IT,IWRITE)                          LES04230
C                                                 LES04240
C-----LES04250
  DOUBLE PRECISION ALPHA(1),BETA(*),V1(1),V2(*),VS(*) LES04260
  DOUBLE PRECISION X1,U,Z,EST,TEMP,TO,T1,RATIO,SUM,XU,NORM,TSUM LES04270
  DOUBLE PRECISION BETAM,EPS,EPS3,EPS4,ZERO,ONE LES04280

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REAL G(1) LES04290
INTEGER MP(1) LES04300
DOUBLE PRECISION FINPRO LES04310
REAL ABS LES04320
DOUBLE PRECISION DABS, DMIN1, DSQRT, DFLOAT LES04330
C-----LES04340
C COMPUTES ERROR ESTIMATES FOR COMPUTED ISOLATED GOOD T-EIGENVALUES LES04350
C IN VS AND WRITES THESE T-EIGENVALUES AND ESTIMATES TO FILE 4. LES04360
C BY DEFINITION A GOOD T-EIGENVALUE IS ISOLATED IF ITS LES04370
C CLOSEST T-NEIGHBOR IS ALSO GOOD, OR ITS CLOSEST NEIGHBOR IS LES04380
C SPURIOUS, BUT THAT NEIGHBOR IS FAR ENOUGH AWAY. SO LES04390
C IN PARTICULAR, WE COMPUTE ESTIMATES FOR GOOD T-EIGENVALUES LES04400
C THAT ARE IN CLUSTERS OF GOOD T-EIGENVALUES. LES04410
C LES04420
C USES INVERSE ITERATION ON T(1,MEV) SOLVING THE EQUATION LES04430
C (T - X1*I)V2 = RIGHT-HAND SIDE (RANDOMLY-GENERATED) LES04440
C FOR EACH SUCH GOOD T-EIGENVALUE X1. LES04450
C LES04460
C PROGRAM REFACTORS T-X1*I ON EACH ITERATION OF INVERSE ITERATION. LES04470
C TYPICALLY ONLY ONE ITERATION IS NEEDED PER EIGENVALUE X1. LES04480
C LES04490
C POSSIBLE STORAGE COMPRESSION LES04500
C G STORAGE COULD BE ELIMINATED BY REGENERATING THE RANDOM LES04510
C RIGHT-HAND SIDE ON EACH ITERATION AND PRINTING OUT THE LES04520
C ERROR ESTIMATES AS THEY ARE GENERATED. LES04530
C LES04540
C ON ENTRY AND EXIT LES04550
C MEV = ORDER OF T LES04560
C ALPHA, BETA CONTAIN THE NONZERO ENTRIES OF THE T-MATRIX LES04570
C VS = COMPUTED DISTINCT EIGENVALUES OF T(1,MEV) LES04580
C MP = T-MULTIPLICITY OF EACH T-EIGENVALUE IN VS. MP(I) = -1 MEANS LES04590
C VS(I) IS A GOOD T-EIGENVALUE BUT THAT IT IS SITTING CLOSE TO LES04600
C A SPURIOUS T-EIGENVALUE. MP(I) = 0 MEANS VS(I) IS SPURIOUS. LES04610
C ESTIMATES ARE COMPUTED ONLY FOR THOSE T-EIGENVALUES LES04620
C WITH MP(I) = 1. FLAGGING WAS DONE IN SUBROUTINE ISOEV LES04630
C PRIOR TO ENTERING INVERR. LES04640
C NISO = NUMBER OF ISOLATED GOOD T-EIGENVALUES CONTAINED IN VS LES04650
C NDIS = NUMBER OF DISTINCT T-EIGENVALUES IN VS LES04660
C IKL = SEED FOR RANDOM NUMBER GENERATOR LES04670
C EPS = 2. * MACHINE EPSILON LES04680
C LES04690
C IN PROGRAM: LES04700
C ITER = MAXIMUM NUMBER OF INVERSE ITERATION STEPS ALLOWED FOR EACH LES04710
C X1. ITER = IT ON ENTRY. LES04720
C G = ARRAY OF DIMENSION AT LEAST MEV + NISO. USED TO STORE LES04730
C RANDOMLY-GENERATED RIGHT-HAND SIDE. THIS IS NOT LES04740
C REGENERATED FOR EACH X1. G IS ALSO USED TO STORE ERROR LES04750
C ESTIMATES AS THEY ARE COMPUTED FOR LATER PRINTOUT. LES04760
C V1,V2 = WORK SPACES USED IN THE FACTORIZATION OF T(1,MEV). LES04770
C AT THE END OF THE INVERSE ITERATION COMPUTATION FOR X1, V2 LES04780
C CONTAINS THE UNIT EIGENVECTOR OF T(1,MEV) CORRESPONDING TO X1. LES04790
C V1 AND V2 MUST BE OF DIMENSION AT LEAST MEV. LES04800
C LES04810
C ON EXIT LES04820
C G(J) = MINIMUM GAP IN T(1,MEV) FOR EACH VS(J), J=1,NDIS LES04830

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C      G(MEV+I) = BETAM*|V2(MEV)| = ERROR ESTIMATE FOR ISOLATED GOOD      LES04840
C      T-EIGENVALUES, WHERE I = 1,NISO AND BETAM = BETA(MEV+1) LES04850
C      V2(MEV) IS LAST COMPONENT OF THE UNIT EIGENVECTOR OF      LES04860
C      T(1,MEV) CORRESPONDING TO ITH ISOLATED GOOD T-EIGENVALUE. LES04870
C                                                                    LES04880
C      IF FOR SOME X1 IT.GT.ITER THEN THE ERROR ESTIMATE IN G IS MARKED LES04890
C      WITH A - SIGN.      LES04900
C                                                                    LES04910
C      V2 = ISOLATED GOOD T-EIGENVALUES      LES04920
C      V1 = MINIMAL T-GAPS FOR THE T-EIGENVALUES IN V2.      LES04930
C      THESE ARE CONSTRUCTED FOR WRITE-OUT PURPOSES ONLY AND NOT      LES04940
C      NEEDED ELSEWHERE IN THE PROGRAM.      LES04950
C-----LES04960
C                                                                    LES04970
C      LABEL OUTPUT FILE 4      LES04980
C      IF (MMB.EQ.1) WRITE(4,10)      LES04990
10  FORMAT(' INVERSE ITERATION ERROR ESTIMATES'/)      LES05000
C                                                                    LES05010
C      FILE 6 (TERMINAL) OUTPUT OF ERROR ESTIMATES      LES05020
C      IF (IWRITE.NE.0.AND.NISO.NE.0) WRITE(6,20)      LES05030
20  FORMAT('/ INVERSE ITERATION ERROR ESTIMATES'/ ' JISO', ' JDIST',8X LES05040
1, 'GOOD T-EIGENVALUE',4X, 'BETAM*UM',5X, 'TMINGAP')      LES05050
C                                                                    LES05060
C      INITIALIZATION AND PARAMETER SPECIFICATION      LES05070
C      ZERO = 0.ODO      LES05080
C      ONE = 1.ODO      LES05090
C      NG = 0      LES05100
C      NISO = 0      LES05110
C      ITER = IT      LES05120
C      MP1 = MEV+1      LES05130
C      MM1 = MEV-1      LES05140
C      BETAM = BETA(MP1)      LES05150
C      BETA(MP1) = ZERO      LES05160
C                                                                    LES05170
C      CALCULATE SCALE AND TOLERANCES      LES05180
C      TSUM = DABS(ALPHA(1))      LES05190
C      DO 30 I = 2,MEV      LES05200
30  TSUM = TSUM + DABS(ALPHA(I)) + BETA(I)      LES05210
C                                                                    LES05220
C      EPS3 = EPS*TSUM      LES05230
C      EPS4 = DFLOAT(MEV)*EPS3      LES05240
C                                                                    LES05250
C      GENERATE SCALED RANDOM RIGHT-HAND SIDE      LES05260
C      ILL = IKL      LES05270
C                                                                    LES05280
C-----LES05290
C      CALL GENRAN(ILL,G,MEV)      LES05300
C-----LES05310
C                                                                    LES05320
C      GSUM = ZERO      LES05330
C      DO 40 I = 1,MEV      LES05340
40  GSUM = GSUM+ABS(G(I))      LES05350
C      GSUM = EPS4/GSUM      LES05360
C                                                                    LES05370
C      DO 50 I = 1,MEV      LES05380

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50 G(I) = GSUM*G(I) LES05390
C LES05400
C LOOP ON ISOLATED GOOD T-EIGENVALUES IN VS (MP(I) = 1) TO LES05410
C CALCULATE CORRESPONDING UNIT EIGENVECTOR OF T(1,MEV) LES05420
C LES05430
C DO 180 JEV = 1,NDIS LES05440
C LES05450
C IF (MP(JEV).EQ.0) GO TO 180 LES05460
C NG = NG + 1 LES05470
C IF (MP(JEV).NE.1) GO TO 180 LES05480
C LES05490
C IT = 1 LES05500
C NISO = NISO + 1 LES05510
C X1 = VS(JEV) LES05520
C LES05530
C INITIALIZE RIGHT HAND SIDE FOR INVERSE ITERATION LES05540
C DO 60 I = 1,MEV LES05550
60 V2(I) = G(I) LES05560
C LES05570
C TRIANGULAR FACTORIZATION WITH NEAREST NEIGHBOR PIVOT LES05580
C STRATEGY. INTERCHANGES ARE LABELLED BY SETTING BETA < 0. LES05590
C LES05600
70 CONTINUE LES05610
C U = ALPHA(1)-X1 LES05620
C Z = BETA(2) LES05630
C LES05640
C DO 90 I = 2,MEV LES05650
C IF (BETA(I).GT.DABS(U)) GO TO 80 LES05660
C NO INTERCHANGE LES05670
C V1(I-1) = Z/U LES05680
C V2(I-1) = V2(I-1)/U LES05690
C V2(I) = V2(I)-BETA(I)*V2(I-1) LES05700
C RATIO = BETA(I)/U LES05710
C U = ALPHA(I)-X1-Z*RATIO LES05720
C Z = BETA(I+1) LES05730
C GO TO 90 LES05740
80 CONTINUE LES05750
C INTERCHANGE CASE LES05760
C RATIO = U/BETA(I) LES05770
C BETA(I) = -BETA(I) LES05780
C V1(I-1) = ALPHA(I)-X1 LES05790
C U = Z-RATIO*V1(I-1) LES05800
C Z = -RATIO*BETA(I+1) LES05810
C TEMP = V2(I-1) LES05820
C V2(I-1) = V2(I) LES05830
C V2(I) = TEMP-RATIO*V2(I) LES05840
90 CONTINUE LES05850
C IF (U.EQ.ZERO) U = EPS3 LES05860
C LES05870
C SMALLNESS TEST AND DEFAULT VALUE FOR LAST COMPONENT LES05880
C PIVOT(I-1) = |BETA(I)| FOR INTERCHANGE CASE LES05890
C (I-1,I+1) ELEMENT IN RIGHT FACTOR = BETA(I+1) LES05900
C END OF FACTORIZATION AND FORWARD SUBSTITUTION LES05910
C LES05920
C BACK SUBSTITUTION LES05930

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WRITE(6,170) NISO,JEV,X1,EST,GAP
170 FORMAT(2I6,E25.16,2E12.3)
C
180 CONTINUE
C
C END ERROR ESTIMATE LOOP ON ISOLATED GOOD T-EIGENVALUES.
C GENERATE DISTINCT MINGAPS FOR T(1,MEV). THIS IS USEFUL AS AN
C INDICATOR OF THE GOODNESS OF THE INVERSE ITERATION ESTIMATES.
C TRANSFER ISOLATED GOOD T-EIGENVALUES AND CORRESPONDING TMINGAPS
C TO V2 AND V1 FOR OUTPUT PURPOSES ONLY.
C
NM1 = NDIS - 1
G(NDIS) = VS(NM1)-VS(NDIS)
G(1) = VS(2)-VS(1)
C
DO 190 J = 2,NM1
TO = VS(J)-VS(J-1)
T1 = VS(J+1)-VS(J)
G(J) = T1
IF (TO.LT.T1) G(J)=-TO
190 CONTINUE
ISO = 0
DO 200 J = 1,NDIS
IF (MP(J).NE.1) GO TO 200
ISO = ISO+1
V1(ISO) = G(J)
V2(ISO) = VS(J)
200 CONTINUE
C
IF(NISO.EQ.0) GO TO 250
C
C ERROR ESTIMATES ARE WRITTEN TO FILE 4
WRITE(4,210)MEV,NDIS,NG,NISO,N,IKL,ITER,BETAM
210 FORMAT(1X,'TSIZE',2X,'NDIS',1X,'NGOOD',2X,'NISO',1X,'ASIZE'/5I6/
1 4X,'RHSEED',2X,'MXINIT',5X,'BETAM'/I10,I8,E10.3/
2 2X,'GOODEVNO',8X,'GOOD T-EIGENVALUE',6X,'BETAM*UM',7X,'TMINGAP')
C
ISPUR = 0
I = 0
DO 240 J = 1,NDIS
IF(MP(J).NE.0) GO TO 220
ISPUR = ISPUR + 1
GO TO 240
220 IF(MP(J).NE.1) GO TO 240
I = I + 1
MEVI = MEV + I
IGOOD = J - ISPUR
WRITE(4,230) IGOOD,V2(I),G(MEVI),V1(I)
230 FORMAT(I10,E25.16,2E14.3)
240 CONTINUE
GO TO 270
C
250 WRITE(4,260)
260 FORMAT(/' THERE ARE NO ISOLATED T-EIGENVALUES SO NO ERROR ESTIMATELES07020
1S WERE COMPUTED')

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C                                                    LES07040
C   RESTORE BETA(MEV+1) = BETAM                      LES07050
C   270 BETA(MP1) = BETAM                            LES07060
C-----END OF INVERR-----LES07070
C   RETURN                                           LES07080
C   END                                              LES07090
C                                                    LES07100
C-----START OF TNORM-----LES07110
C                                                    LES07120
C   SUBROUTINE TNORM(ALPHA,BETA,BMIN,TMAX,MEV,IB)     LES07130
C                                                    LES07140
C-----LES07150
C   DOUBLE PRECISION ALPHA(1),BETA(*)                LES07160
C   DOUBLE PRECISION TMAX,BMIN,BMAX,BSIZE,BTOL       LES07170
C   DOUBLE PRECISION DABS, DMAX1                     LES07180
C-----LES07190
C   COMPUTE SCALING FACTOR USED IN THE T-MULTIPLICITY, SPURIOUS AND LES07200
C   PRTESTS. CHECK RELATIVE SIZE OF THE BETA(K), K=1,MEV LES07210
C   AS A TEST ON THE LOCAL ORTHOGONALITY OF THE LANCZOS VECTORS. LES07220
C                                                    LES07230
C   TMAX = MAX (|ALPHA(I)|, BETA(I), I=1,MEV)         LES07240
C   BMIN = MIN (BETA(I) I=2,MEV)                     LES07250
C   BSIZE = BMIN/TMAX                                 LES07260
C   |IB| = INDEX OF MINIMAL(BETA)                    LES07270
C   IB < 0 IF BMIN/TMAX < BTOL                       LES07280
C-----LES07290
C   SPECIFY PARAMETERS                                LES07300
C   IB = 2                                            LES07310
C   BTOL = BMIN                                       LES07320
C   BMIN = BETA(2)                                     LES07330
C   BMAX = BETA(2)                                     LES07340
C   TMAX = DABS(ALPHA(1))                             LES07350
C                                                    LES07360
C   DO 20 I = 2,MEV                                   LES07370
C   IF (BETA(I).GE.BMIN) GO TO 10                     LES07380
C   IB = I                                            LES07390
C   BMIN = BETA(I)                                    LES07400
C 10 TMAX = DMAX1(TMAX,DABS(ALPHA(I)))                 LES07410
C   BMAX = DMAX1(BETA(I),BMAX)                       LES07420
C 20 CONTINUE                                         LES07430
C   TMAX = DMAX1(BMAX,TMAX)                           LES07440
C                                                    LES07450
C   TEST OF LOCAL ORTHOGONALITY USING SCALED BETAS LES07460
C   BSIZE = BMIN/TMAX                                 LES07470
C   IF (BSIZE.GE.BTOL) GO TO 40                      LES07480
C                                                    LES07490
C   DEFAULT. BSIZE IS SMALLER THAN TOLERANCE BTOL SPECIFIED IN MAIN LES07500
C   PROGRAM. PROGRAM TERMINATES FOR USER TO DECIDE WHAT TO DO LES07510
C   BECAUSE LOCAL ORTHOGONALITY OF THE LANCZOS VECTORS COULD BE LES07520
C   LOST.                                             LES07530
C                                                    LES07540
C   IB = -IB                                          LES07550
C   WRITE(6,30) MEV                                   LES07560
C 30 FORMAT(/' BETA TEST INDICATES POSSIBLE LOSS OF LOCAL ORTHOGONALITYLES07570
C   1OVER 1ST',I6,' LANCZOS VECTORS'/)                LES07580

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C LES07590
40 CONTINUE LES07600
C LES07610
  WRITE(6,50) IB LES07620
50 FORMAT(/' MINIMUM BETA RATIO OCCURS AT',I6,' TH BETA'/) LES07630
C LES07640
  WRITE(6,60) MEV,BMIN,TMAX,BSIZE LES07650
60 FORMAT(/1X,'TSIZE',6X,'MIN BETA',5X,'TKMAX',6X,'MIN RATIO'/ LES07660
  1 I6,E14.3,E10.3,E15.3/) LES07670
C LES07680
C-----END OF TNORM-----LES07690
  RETURN LES07700
  END LES07710
C LES07720
C LES07730
C-----START OF LUMP-----LES07740
C LES07750
  SUBROUTINE LUMP(V1,RELTOL,MULTOL,SCALE2,LINDEX,LOOP) LES07760
C LES07770
C-----LES07780
  DOUBLE PRECISION V1(1),SUM,RELTOL,MULTOL,THOLD,ZERO,SCALE2 LES07790
  INTEGER LINDEX(1) LES07800
  DOUBLE PRECISION DABS,DFLOAT,DMAX1 LES07810
C-----LES07820
C LINDEX(J) = T-MULTIPLICITY OF JTH DISTINCT T-EIGENVALUE LES07830
C LOOP = NUMBER OF DISTINCT T-EIGENVALUES LES07840
C LUMP 'COMBINES' COMPUTED 'GOOD' T-EIGENVALUES THAT ARE LES07850
C 'TOO CLOSE'. LES07860
C VALUE OF RELTOL IS 1.D-10. LES07870
C LES07880
C IF IN A SET OF T-EIGENVALUES TO BE COMBINED THERE IS AN EIGENVALUELES07890
C WITH LINDEX=1, THEN THE VALUE OF THE COMBINED EIGENVALUES IS SET LES07900
C EQUAL TO THE VALUE OF THAT EIGENVALUE. NOTE THAT IF A SPURIOUS LES07910
C T-EIGENVALUE IS TO BE 'COMBINED' WITH A GOOD T-EIGENVALUE, THEN LES07920
C THIS IS DONE ONLY BY INCREASING THE INDEX, LINDEX, FOR THAT LES07930
C T-EIGENVALUE. NUMERICAL VALUES OF SPURIOUS EIGENVALUES ARE NEVER LES07940
C COMBINE WITH THOSE OF GOOD T-EIGENVALUES. LES07950
C-----LES07960
  ZERO = 0.0D0 LES07970
  NLOOP = 0 LES07980
  J = 0 LES07990
  ICOUNT = 1 LES08000
  JI = 1 LES08010
  THOLD = DMAX1(RELTOL*DABS(V1(1)),SCALE2*MULTOL) LES08020
C THOLD = DMAX1(RELTOL*DABS(V1(1)),RELTOL) LES08030
C LES08040
10 J = J+1 LES08050
  IF (J.EQ.LOOP) GO TO 20 LES08060
  SUM = DABS(V1(J)-V1(J+1)) LES08070
  IF (SUM.LT.THOLD) GO TO 60 LES08080
20 JF = JI + ICOUNT - 1 LES08090
  INDSUM = 0 LES08100
  ISPUR = 0 LES08110
C LES08120
DO 30 KK = JI,JF LES08130

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C-----START OF ISOEV-----LES08690
C                                     LES08700
      SUBROUTINE ISOEV(VS,GAPTOL,MULTOL,SCALE1,G,MP,NDIS,NG,NISO)   LES08710
C                                     LES08720
C-----LES08730
      DOUBLE PRECISION  VS(*),T0,T1,MULTOL,GAPTOL,SCALE1,TEMP     LES08740
      REAL  G(1),GAP                                             LES08750
      INTEGER  MP(1)                                           LES08760
      REAL  ABS                                                  LES08770
      DOUBLE PRECISION  DABS, DMAX1                             LES08780
C-----LES08790
C  GENERATE DISTINCT TMINGAPS AND USE THEM TO LABEL THE ISOLATED  LES08800
C  GOOD T-EIGENVALUES THAT ARE VERY CLOSE TO SPURIOUS ONES.     LES08810
C  ERROR ESTIMATES WILL NOT BE COMPUTED FOR THESE T-EIGENVALUES. LES08820
C                                     LES08830
C  ON ENTRY AND EXIT                                             LES08840
C  VS CONTAINS THE COMPUTED DISTINCT EIGENVALUES OF T(1,MEV)    LES08850
C  MP CONTAINS THE CORRESPONDING T-MULTIPLICITIES               LES08860
C  NDIS = NUMBER OF DISTINCT EIGENVALUES                         LES08870
C  GAPTOL = RELATIVE GAP TOLERANCE SET IN MAIN                  LES08880
C                                     LES08890
C  ON EXIT                                                        LES08900
C  G CONTAINS THE TMINGAPS.                                     LES08910
C  G(I) < 0 MEANS MINGAP IS DUE TO LEFT GAP                     LES08920
C  MP(I) IS NOT CHANGED EXCEPT THAT  MP(I)=-1, IF MP(I)=1,   LES08930
C  TMINGAP WAS TOO SMALL AND DUE TO A SPURIOUS T-EIGENVALUE.  LES08940
C                                     LES08950
C  IF MP(I)=-1 THAT SIMPLE GOOD T-EIGENVALUE WILL BE SKIPPED  LES08960
C  IN THE SUBSEQUENT ERROR ESTIMATE COMPUTATIONS IN INVERR     LES08970
C  THAT IS, WE COMPUTE ERROR ESTIMATES ONLY FOR THOSE GOOD    LES08980
C  T-EIGENVALUES WITH MP(I)=1.                                  LES08990
C-----LES09000
C  CALCULATE MINGAPS FOR DISTINCT T(1,MEV) EIGENVALUES.        LES09010
      NM1 = NDIS - 1                                           LES09020
      G(NDIS) = VS(NM1)-VS(NDIS)                               LES09030
      G(1) = VS(2)-VS(1)                                       LES09040
C                                     LES09050
      DO 10 J = 2,NM1                                          LES09060
      TO = VS(J)-VS(J-1)                                       LES09070
      T1 = VS(J+1)-VS(J)                                       LES09080
      G(J) = T1                                                 LES09090
      IF (TO.LT.T1) G(J) = -TO                                  LES09100
10  CONTINUE                                                  LES09110
C                                     LES09120
C  SET MP(I)=-1 FOR SIMPLE GOOD T-EIGENVALUES WHOSE MINGAPS  ARE LES09130
C  'TOO SMALL' AND DUE TO SPURIOUS T-EIGENVALUES.             LES09140
C                                     LES09150
      NISO = 0                                                 LES09160
      NG = 0                                                   LES09170
      DO 20 J = 1,NDIS                                         LES09180
      IF (MP(J).EQ.0) GO TO 20                                  LES09190
      NG = NG+1                                                LES09200
      IF (MP(J).NE.1) GO TO 20                                  LES09210
C  VS(J) IS NEXT SIMPLE GOOD T-EIGENVALUE                     LES09220
      NISO = NISO + 1                                          LES09230

```

```

I = J+1
IF (G(J).LT.0.0) I = J-1
IF (MP(I).NE.0) GO TO 20
GAP = ABS(G(J))
TO = DMAX1(SCALE1*MULTOL,GAPTOL*DABS(VS(J)))
C TO = DMAX1(GAPTOL,GAPTOL*DABS(VS(J)))
TEMP = TO
IF (GAP.GT.TEMP) GO TO 20
MP(J) = -MP(J)
NISO = NISO-1
20 CONTINUE
C
C-----END OF ISOEV-----
RETURN
END
C
C-----START OF PRTEST-----
C
SUBROUTINE PRTEST(ALPHA,BETA,TEIG,TKMAX,EPSM,RELTOL,SCALE3,SCALE4,
1 TMULT,NDIST,MEV,I PROJ)
C
C-----
DOUBLE PRECISION ALPHA(1), BETA(1),TEIG(*),SIGMA(10)
DOUBLE PRECISION EPSM,RELTOL,PRTOL,TKMAX,LRATIO,URATIO
DOUBLE PRECISION EPS,EPS1,BETAM,LBD,UBD,SIG,YU,YV,LRATS,URATS
DOUBLE PRECISION ZERO,ONE,TEN,BISTOL,SCALE3,SCALE4,AEV,TEMP
INTEGER TMULT(*),ISIGMA(10)
DOUBLE PRECISION DABS, DMAX1, DSQRT, DFLOAT
C-----
C AFTER CONVERGENCE HAS BEEN ESTABLISHED, SUBROUTINE PRTEST
C TESTS COMPUTED EIGENVALUES OF T(1,MEV) THAT HAVE BEEN LABELLED
C SPURIOUS TO DETERMINE IF ANY EIGENVALUES OF A HAVE BEEN
C MISSED BY LANCZOS PROCEDURE. AN EIGENVALUE WITH A VERY SMALL
C PROJECTION ON THE STARTING VECTOR (< SINGLE PRECISION)
C CAN BE MISSED BECAUSE IT IS ALSO AN EIGENVALUE OF T(2,MEV) TO
C WITHIN THE SQUARE OF THIS ORIGINAL PROJECTION.
C OUR EXPERIENCE IS THAT SUCH SMALL PROJECTIONS OCCUR ONLY
C VERY INFREQUENTLY.
C
C THIS SUBROUTINE IS CALLED ONLY AFTER CONVERGENCE HAS BEEN
C ESTABLISHED. ONCE CONVERGENCE HAS BEEN OBSERVED ON THE
C OTHER EIGENVALUES THEN ONE CAN EXPECT TO ALSO HAVE CONVERGENCE
C ON ANY SUCH HIDDEN EIGENVALUES.(IF THERE ARE ANY). THIS
C PROCEDURE CONSIDERS ONLY SPURIOUS T-EIGENVALUES AND ONLY THOSE
C SPURIOUS T-EIGENVALUES THAT ARE ISOLATED FROM GOOD T-EIGENVALUES.
C FOR EACH SUCH T-EIGENVALUE IT DOES 2 STURM SEQUENCES
C AND A FEW SCALAR MULTIPLICATIONS. UPON RETURN TO MAIN
C PROGRAM ERROR ESTIMATES WILL BE COMPUTED FOR ANY EIGENVALUES
C THAT HAVE BEEN LABELLED AS 'HIDDEN'. SUCH T-EIGENVALUES
C WILL BE RELABELLED AS 'GOOD' ONLY IF THESE ERROR ESTIMATES
C ARE SUFFICIENTLY SMALL.
C-----
ZERO = 0.0DO
ONE = 1.0DO
TEN = 10.0DO

```



```

      PRTOL = 1.D-6                                LES09790
      TEMP = DFLOAT(MEV+1000)                       LES09800
      TEMP = DSQRT(TEMP)                             LES09810
      BISTOL = TKMAX*EPSM*TEMP                       LES09820
      NSIGMA = 4                                     LES09830
      SIGMA(1) = TEN*TKMAX                           LES09840
C
      DO 10 J = 2,NSIGMA                             LES09850
10  SIGMA(J) = TEN*SIGMA(J-1)                       LES09860
C
      IFIN = 0                                       LES09880
      MF = 1                                         LES09890
      ML = MEV                                       LES09900
      BETAM = BETA(MF)                               LES09910
      BETA(MF) = ZERO                                LES09920
      IPROJ = 0                                      LES09930
      J = 1                                          LES09940
C
      IF (TMULT(1).NE.0) GO TO 110                   LES09950
C
      AEV = DABS(TEIG(1))                            LES09960
      TEMP = PRTOL*AEV                              LES09970
      EPS1 = DMAX1(TEMP,SCALE4*BISTOL)               LES09980
C
      EPS1 = DMAX1(TEMP,PRTOL)                       LES09990
      TEMP = RELTOL*AEV                             LES10000
      EPS = DMAX1(TEMP,SCALE3*BISTOL)               LES10010
C
      EPS = DMAX1(TEMP,RELTOL)                       LES10020
C
      IF (TEIG(2)-TEIG(1).LT.EPS1.AND.TMULT(2).NE.0) GO TO 110 LES10030
C
20  LBD = TEIG(J) - EPS                             LES10040
      UBD = TEIG(J) + EPS                             LES10050
      MEVL = 0                                       LES10060
      IL = 0                                         LES10070
      YU = ONE                                       LES10080
C
      DO 50 I=MF,ML                                 LES10090
      IF (YU.NE.ZERO) GO TO 30                       LES10100
      YV = BETA(I)/EPSM                              LES10110
      GO TO 40                                       LES10120
30  YV = BETA(I)*BETA(I)/YU                         LES10130
40  YU = ALPHA(I)-LBD-YV                            LES10140
      IF (YU.GE.ZERO) GO TO 50                       LES10150
C
      MEVL INCREMENTED                              LES10160
      MEVL = MEVL + 1                                LES10170
      IL = I                                         LES10180
50  CONTINUE                                       LES10190
C
      LRATIO = YU                                    LES10200
      MEV1L = MEVL                                  LES10210
      IF (IL.EQ.ML) MEV1L=MEVL-1                    LES10220
C
      MEVL = NUMBER OF EVS OF T(1,MEV) WHICH ARE < LBD LES10230
C
      MEV1L = NUMBER OF EVS OF T(1,MEV-1) WHICH ARE < LBD LES10240
C
      LRATIO = DET(T(1,MEV)-LBD)/DET(T(1,MEV-1)-LBD): LES10250

```

C		LES10340
	MEVU = 0	LES10350
	IL = 0	LES10360
	YU = ONE	LES10370
C		LES10380
	DO 80 I=MF,ML	LES10390
	IF (YU.NE.ZERO) GO TO 60	LES10400
	YV = BETA(I)/EPSM	LES10410
	GO TO 70	LES10420
60	YV = BETA(I)*BETA(I)/YU	LES10430
70	YU = ALPHA(I)-UBD-YV	LES10440
	IF (YU.GE.ZERO) GO TO 80	LES10450
C	MEVU INCREMENTED	LES10460
	MEVU = MEVU + 1	LES10470
	IL = I	LES10480
80	CONTINUE	LES10490
C		LES10500
	URATIO = YU	LES10510
	MEV1U = MEVU	LES10520
	IF (IL.EQ.ML) MEV1U=MEVU-1	LES10530
C		LES10540
C	MEVU = NUMBER OF EVS OF T(MEV) WHICH ARE < UBD	LES10550
C	MEV1U = NUMBER OF EVS OF T(MEV-1) WHICH ARE < UBD	LES10560
C	URATIO = DET(TM-UBD)/DET(T(M-1)-UBD): TM=T(MF,ML)	LES10570
C		LES10580
	NEV1 = MEV1U-MEV1L	LES10590
C		LES10600
	DO 90 K=1,NSIGMA	LES10610
	SIG = SIGMA(K)	LES10620
	LRATS = LRATIO-SIG	LES10630
	URATS = URATIO-SIG	LES10640
C	NOTE THE INCREMENT IS ON NUMBER OF EVALUES OF T(M-1)	LES10650
	MEVLS = MEV1L	LES10660
	IF (LRATS.LT.0.) MEVLS=MEV1L+1	LES10670
	MEVUS = MEV1U	LES10680
	IF (URATS.LT.0.) MEVUS=MEV1U+1	LES10690
	ISIGMA(K) = MEVUS - MEVLS	LES10700
90	CONTINUE	LES10710
C		LES10720
	ICOUNT = 0	LES10730
	DO 100 K=1,NSIGMA	LES10740
100	IF (ISIGMA(K).EQ.1) ICOUNT=ICOUNT + 1	LES10750
C		LES10760
	IF (ICOUNT.LT.2.OR.NEV1.EQ.0) GO TO 110	LES10770
	TMULT(J) = -10	LES10780
	IPROJ=IPROJ+1	LES10790
C		LES10800
110	J=J+1	LES10810
C		LES10820
	IF (J.GE.NDIST) GO TO 120	LES10830
	IF (TMULT(J).NE.0) GO TO 110	LES10840
C		LES10850
	AEV = DABS(TEIG(J))	LES10860
	TEMP = PRTOL*AEV	LES10870
	EPS1 = DMAX1(TEMP,SCALE4*BISTOL)	LES10880

```

C      EPS1 = DMAX1(TEMP,PRTOL)                                LES10890
      TEMP = RELTOL*AEV                                        LES10900
      EPS  = DMAX1(TEMP,SCALE3*BISTOL)                       LES10910
C      EPS  = DMAX1(TEMP,RELTOL)                             LES10920
C                                                                 LES10930
      IF (TEIG(J)-TEIG(J-1).LT.EPS1.AND.TMULT(J-1).NE.0) GO TO 110 LES10940
      IF (TEIG(J+1)-TEIG(J).LT.EPS1.AND.TMULT(J+1).NE.0) GO TO 110 LES10950
C                                                                 LES10960
      GO TO 20                                               LES10970
C                                                                 LES10980
120 IF (IFIN.EQ.1) GO TO 130                                  LES10990
      IF (TMULT(NDIST).NE.0) GO TO 130                       LES11000
C                                                                 LES11010
      AEV = DABS(TEIG(NDIST))                                LES11020
      TEMP = PRTOL*AEV                                       LES11030
      EPS1 = DMAX1(TEMP,SCALE4*BISTOL)                       LES11040
C      EPS1 = DMAX1(TEMP,PRTOL)                              LES11050
      TEMP = RELTOL*AEV                                       LES11060
      EPS  = DMAX1(TEMP,SCALE3*BISTOL)                       LES11070
C      EPS  = DMAX1(TEMP,RELTOL)                             LES11080
C                                                                 LES11090
      NDIST1=NDIST -1                                       LES11100
      TEMP = TEIG(NDIST)-TEIG(NDIST1)                       LES11110
      IF (TEMP.LT.EPS1.AND.TMULT(NDIST1).NE.0) GO TO 130   LES11120
      IFIN = 1                                               LES11130
C                                                                 LES11140
      GO TO 20                                               LES11150
C                                                                 LES11160
130 BETA(MF) = BETAM                                        LES11170
C                                                                 LES11180
C-----END OF PRTEST-----LES11190
      RETURN                                                LES11200
      END                                                    LES11210
C                                                                 LES11220
C-----START OF STURMI-----LES11230
C                                                                 LES11240
      SUBROUTINE STURMI(ALPHA,BETA,X1,TOLN,EPSM,MMAX,MK1,MK2,IC,IWRITE) LES11250
C                                                                 LES11260
C-----LES11270
      DOUBLE PRECISION ALPHA(1),BETA(1)                    LES11280
      DOUBLE PRECISION EPSM,X1,TOLN,EVL,EVU,BETA2          LES11290
      DOUBLE PRECISION U1,U2,V1,V2,ZERO,ONE                LES11300
      INTEGER I,IC,ICD,IC0,IC1,IC2,MK1,MK2,MMAX            LES11310
C-----LES11320
C                                                                 LES11330
C      FOR ANY EIGENVALUE OF A THAT HAS CONVERGED AS AN EIGENVALUE LES11340
C      OF THE T-MATRICES THIS SUBROUTINE CALCULATES        LES11350
C      THE SMALLEST SIZE OF THE T-MATRIX, T(1,MK1) DEFINED LES11360
C      BY THE ALPHA AND BETA ARRAYS SUCH THAT MK1.LE.MMAX  LES11370
C      AND THE INTERVAL (X1-TOLN,X1+TOLN) CONTAINS AT LEAST ONE LES11380
C      EIGENVALUE OF T(1,MK1). IT ALSO CALCULATES MK2 <= MMAX LES11390
C      AS THE SMALLEST SIZE T-MATRIX (IF ANY) SUCH THAT THIS INTERVAL LES11400
C      CONTAINS AT LEAST TWO EIGENVALUES OF T(1,MK2).     LES11410
C      IF NO T-MATRIX OF ORDER < MMAX SATISFIES THIS REQUIREMENT LES11420
C      THEN MK2 IS SET EQUAL TO MMAX. THE EIGENVECTOR PROGRAM LES11430

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        ICO = ICO+1                                LES11990
        IF (ICO.GT.1) GO TO 70                      LES12000
60 CONTINUE                                       LES12010
C                                                LES12020
        I = I-1                                    LES12030
        IF (ICO.EQ.0) MK1 = MMAX                   LES12040
70 MK2 = I                                        LES12050
        IC = ICD                                   LES12060
C                                                LES12070
        IF (IWRITE.EQ.1) WRITE(6,80) X1,MK1,MK2,IC LES12080
80 FORMAT(' EVAL =',E20.12,' MK1 =',I6,' MK2 =',I6,' IC =',I3/) LES12090
C                                                LES12100
        RETURN                                     LES12110
C-----END OF STURMI-----LES12120
        END                                       LES12130
C                                                LES12140
C                                                LES12150
C-----START OF INVERM-----LES12160
C                                                LES12170
        SUBROUTINE INVERM(ALPHA,BETA,V1,V2,X1,ERROR,ERRORV,EPS,G,MEV,IT, LES12180
1 IWRITE)                                       LES12190
C                                                LES12200
C-----LES12210
        DOUBLE PRECISION ALPHA(1),BETA(*),V1(1),V2(*) LES12220
        DOUBLE PRECISION X1,U,Z,TEMP,RATIO,SUM,XU,NORM,TSUM,BETAM LES12230
        DOUBLE PRECISION EPS,EPS3,EPS4,ERROR,ERRORV,ZERO,ONE LES12240
        REAL G(1)                                  LES12250
        DOUBLE PRECISION DABS, DSQRT, DFLOAT LES12260
        DOUBLE PRECISION FINPRO LES12270
        REAL ABS                                    LES12280
C-----LES12290
C                                                LES12300
C COMPUTES T-EIGENVECTORS FOR ISOLATED GOOD T-EIGENVALUES X1 LES12310
C USING INVERSE ITERATION ON T(1,MEV(X1)) SOLVING EQUATION LES12320
C (T - X1*I)V2 = RIGHT-HAND SIDE (RANDOMLY-GENERATED) . LES12330
C PROGRAM REFACTORS T- X1*I ON EACH ITERATION OF INVERSE ITERATION. LES12340
C TYPICALLY ONLY ONE ITERATION IS NEEDED PER T-EIGENVALUE X1. LES12350
C LES12360
C IF IWRITE = 1 THEN THERE ARE EXTENDED WRITES TO FILE 6 (TERMINAL) LES12370
C LES12380
C ON ENTRY G CONTAINS A REAL*4 RANDOM VECTOR WHICH WAS GENERATED LES12390
C IN MAIN PROGRAM. LES12400
C LES12410
C ON ENTRY AND EXIT LES12420
C MEV = ORDER OF T LES12430
C ALPHA, BETA CONTAIN THE DIAGONAL AND OFFDIAGONAL ENTRIES OF T. LES12440
C EPS = 2. * MACHINE EPSILON LES12450
C LES12460
C IN PROGRAM: LES12470
C ITER = MAXIMUM NUMBER STEPS ALLOWED FOR INVERSE ITERATION LES12480
C ITER = IT ON ENTRY. LES12490
C V1,V2 = WORK SPACES USED IN THE FACTORIZATION OF T(1,MEV). LES12500
C V1 AND V2 MUST BE OF DIMENSION AT LEAST MEV. LES12510
C LES12520
C ON EXIT LES12530

```



```

        GO TO 60                                LES13090
C      PIVOT INTERCHANGE                        LES13100
50 CONTINUE                                    LES13110
    RATIO = U/BETA(I)                          LES13120
    BETA(I) = -BETA(I)                          LES13130
    V1(I-1) = ALPHA(I)-X1                      LES13140
    U = Z-RATIO*V1(I-1)                        LES13150
    Z = -RATIO*BETA(I+1)                      LES13160
    TEMP = V2(I-1)                             LES13170
    V2(I-1) = V2(I)                            LES13180
    V2(I) = TEMP-RATIO*V2(I)                  LES13190
60 CONTINUE                                    LES13200
C
    IF (U.EQ.ZERO) U=EPS3                      LES13220
C
C      SMALLNESS TEST AND DEFAULT VALUE FOR LAST COMPONENT LES13240
C      PIVOT(I-1) = |BETA(I)| FOR INTERCHANGE CASE LES13250
C      (I-1,I+1) ELEMENT IN RIGHT FACTOR = BETA(I+1) LES13260
C      END OF FACTORIZATION AND FORWARD SUBSTITUTION LES13270
C
C      BACK SUBSTITUTION                        LES13290
    V2(MEV) = V2(MEV)/U                       LES13300
    DO 80 II = 1,MM1                           LES13310
    I = MEV-II                                 LES13320
    IF (BETA(I+1).LT.ZERO) GO TO 70            LES13330
C      NO PIVOT INTERCHANGE                    LES13340
    V2(I) = V2(I)-V1(I)*V2(I+1)               LES13350
    GO TO 80                                    LES13360
C      PIVOT INTERCHANGE                        LES13370
70 BETA(I+1) = -BETA(I+1)                     LES13380
    V2(I) = (V2(I)-V1(I)*V2(I+1)-BETA(I+2)*V2(I+2))/BETA(I+1) LES13390
80 CONTINUE                                    LES13400
C
C
C      TESTS FOR CONVERGENCE OF INVERSE ITERATION LES13430
C      IF SUM |V2| COMPS. LE. 1 AND IT. LE. ITER DO ANOTHER INVIT STEP LES13440
C
    NORM = DABS(V2(MEV))                       LES13460
    DO 90 II = 1,MM1                           LES13470
    I = MEV-II                                 LES13480
90 NORM = NORM+DABS(V2(I))                   LES13490
C
C      IS DESIRED GROWTH IN VECTOR ACHIEVED ? LES13510
C      IF NOT, DO ANOTHER INVERSE ITERATION STEP UNLESS NUMBER ALLOWED IS LES13520
C      EXCEEDED.                               LES13530
    IF (NORM.GE.ONE) GO TO 110                 LES13540
C
    IT=IT+1                                    LES13560
    IF (IT.GT.ITER) GO TO 110                 LES13570
C
    XU = EPS4/NORM                             LES13590
    DO 100 I=1,MEV                             LES13600
100 V2(I) = V2(I)*XU                          LES13610
C
    GO TO 40                                    LES13630

```

```

C                                                    LES13640
C   NORMALIZE COMPUTED T-EIGENVECTOR : V2 = V2/||V2||   LES13650
C                                                    LES13660
110 CONTINUE                                           LES13670
C                                                    LES13680
      SUM = FINPRO(MEV,V2(1),1,V2(1),1)                 LES13690
      SUM = ONE/DSQRT(SUM)                               LES13700
      DO 120 II = 1,MEV                                  LES13710
120  V2(II) = SUM*V2(II)                                LES13720
C                                                    LES13730
C   SAVE ERROR ESTIMATE FOR LATER OUTPUT               LES13740
      ERROR = DABS(V2(MEV))                             LES13750
C                                                    LES13760
C   GENERATE ERRORV = ||T*V2 - X1*V2||.               LES13770
      V1(MEV) = ALPHA(MEV)*V2(MEV)+BETA(MEV)*V2(MEV-1)-X1*V2(MEV) LES13780
      DO 130 J = 2,MM1                                   LES13790
      JM = MP1 - J                                       LES13800
      V1(JM) = ALPHA(JM)*V2(JM) + BETA(JM)*V2(JM-1) + BETA(JM+1)*V2(JM+1) LES13810
      V1(JM) - X1*V2(JM)                                  LES13820
130 CONTINUE                                           LES13830
C                                                    LES13840
      V1(1) = ALPHA(1)*V2(1) + BETA(2)*V2(2) - X1*V2(1) LES13850
      ERRORV = FINPRO(MEV,V1(1),1,V1(1),1)              LES13860
      ERRORV = DSQRT(ERRORV)                             LES13870
      IF (IT.GT.ITER) ERRORV = -ERRORV                  LES13880
      IF (IWRITE.EQ.0) GO TO 150                         LES13890
C                                                    LES13900
C   FILE 6 (TERMINAL) OUTPUT OF ERROR ESTIMATES.      LES13910
      WRITE(6,140) MEV,X1,ERROR,ERRORV                 LES13920
140  FORMAT(2X,'Tsize',15X,'EIGENVALUE',11X,'U(M)',9X,'ERRORV' / LES13930
      1 I6,E25.16,2E15.5)                               LES13940
C                                                    LES13950
C   RESTORE BETA(MEV+1) = BETAM                        LES13960
150 CONTINUE                                           LES13970
      BETA(MP1) = BETAM                                  LES13980
C-----END OF INVERM-----LES13990
      RETURN                                           LES14000
      END                                              LES14010
C                                                    LES14020
C-----START OF LBISEC-----LES14030
C                                                    LES14040
      SUBROUTINE LBISEC(ALPHA,BETA,EPSM,EVAL,EVALN,LB,UB,TTOL,M,NEVT) LES14050
C                                                    LES14060
C-----LES14070
      DOUBLE PRECISION ALPHA(1),BETA(1),X0,X1,XL,XU,YU,YV,LB,UB LES14080
      DOUBLE PRECISION EPSM,EP1,EVAL,EVALN,EVD,EPT     LES14090
      DOUBLE PRECISION ZERO,ONE,HALF,TTOL,TEMP        LES14100
      DOUBLE PRECISION DABS,DSQRT,DFLOAT              LES14110
C-----LES14120
C   SPECIFY PARAMETERS                                  LES14130
      ZERO = 0.0DO                                       LES14140
      HALF = 0.5DO                                       LES14150
      ONE  = 1.0DO                                       LES14160
      XL  = LB                                           LES14170
      XU  = UB                                           LES14180

```



```

C LES14190
C EP1 = DSQRT(1000+M)*TTOL      TTOL = EPSM*TKMAX      LES14200
C TKMAX = MAX(|ALPHA(K)|, BETA(K), K= 1, KMAX)      LES14210
C LES14220
C TEMP = DFLOAT(1000+M)      LES14230
C EP1 = DSQRT(TEMP)*TTOL      LES14240
C LES14250
C NA = 0      LES14260
C X1 = XU      LES14270
C JSTURM = 1      LES14280
C GO TO 60      LES14290
C FORWARD STURM CALCULATION      LES14300
10 NA = NEV      LES14310
C X1 = XL      LES14320
C JSTURM = 2      LES14330
C GO TO 60      LES14340
C FORWARD STURM CALCULATION      LES14350
20 NEVT = NEV      LES14360
C LES14370
C WRITE(6,30) M, EVAL, NEVT, EP1      LES14380
30 FORMAT(/3X, 'T SIZE', 23X, 'EV', 9X/I8, E25.16/      LES14390
1 I6, ' = NUMBER OF T(1,M) EIGENVALUES ON TEST INTERVAL' /      LES14400
1 E12.3, ' = CONVERGENCE TOLERANCE' /)      LES14410
C LES14420
C IF (NEVT.NE.1) GO TO 120      LES14430
C LES14440
C BISECTION LOOP      LES14450
C JSTURM = 3      LES14460
40 X1 = HALF*(XL+XU)      LES14470
C X0 = XU-XL      LES14480
C EPT = EPSM*(DABS(XL) + DABS(XU)) + EP1      LES14490
C CONVERGENCE TEST      LES14500
C IF (X0.LE.EP1) GO TO 100      LES14510
C GO TO 60      LES14520
C FORWARD STURM CALCULATION      LES14530
50 CONTINUE      LES14540
C IF(NEV.EQ.0) XU = X1      LES14550
C IF(NEV.EQ.1) XL = X1      LES14560
C GO TO 40      LES14570
C NEV = NUMBER OF T-EIGENVALUES OF T(1,M) ON (X1,XU)      LES14580
C THERE IS EXACTLY ONE T-EIGENVALUE OF T(1,M) ON (XL,XU)      LES14590
C LES14600
C FORWARD STURM CALCULATION      LES14610
60 NEV = -NA      LES14620
C YU = ONE      LES14630
C DO 90 I = 1, M      LES14640
C IF (YU.NE.ZERO) GO TO 70      LES14650
C YV = BETA(I)/EPSM      LES14660
C GO TO 80      LES14670
70 YV = BETA(I)*BETA(I)/YU      LES14680
80 YU = X1 - ALPHA(I) - YV      LES14690
C IF (YU.GE.ZERO) GO TO 90      LES14700
C NEV = NEV+1      LES14710
90 CONTINUE      LES14720
C GO TO (10,20,50), JSTURM      LES14730

```



```

C-----LES15290
C   IPERM = 1                               LES15300
      DO 10 K = 1,N                          LES15310
        J = IPR(K)                           LES15320
    10 U(K) = W(J)                            LES15330
      GO TO 60                                LES15340
C-----LES15350
C   IPERM = 2                               LES15360
    30 DO 40 K = 1,N                          LES15370
      J = IPT(K)                              LES15380
    40 U(K) = W(J)                            LES15390
C-----LES15400
    60 CONTINUE                               LES15410
      DO 50 K = 1,N                          LES15420
    50 W(K) = U(K)                            LES15430
C                                             LES15440
      4 RETURN                                LES15450
C                                             LES15460
C-----END OF LPERM-----LES15470
      END                                    LES15480

```

## 2.7 LECOMPAC: Optional Preprocessing Program

```

C-----LECOMPAC-(STAND-ALONE PROGRAM)-----LEC00010
C  AUTHOR:   RALPH A. WILLOUGHBY (Deceased)      LEC00020
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C                                                    LEC00070
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C  and modifications of them or portions of them are NOT to be   LEC00090
C  incorporated into any commercial codes or used for any other  LEC00100
C  commercial purposes such as consulting for other companies,    LEC00110
C  without legal agreements with the authors of these Codes.     LEC00120
C  If these Codes or portions of them are used in other scientific or LEC00130
C  engineering research works the names of the authors of these codes LEC00140
C  and appropriate references to their written work are to be     LEC00150
C  incorporated in the derivative works.                          LEC00160
C                                                    LEC00170
C  This header is not to be removed from these codes.            LEC00180
C                                                    LEC00190
C                                                    LEC00200
C  THIS PROGRAM TRANSLATES A SPARSE SYMMETRIC N X N MATRIX A,    LEC00210
C  GIVEN AS I, J, A(I,J), INTO THE SPARSE MATRIX FORMAT          LEC00220
C  REQUIRED BY THE SAMPLE USPEC AND CMATV PROGRAMS PROVIDED        LEC00230
C  FOR USE WITH THE LANCZOS EIGENVALUE/EIGENVECTOR PROCEDURES.   LEC00240
C  THIS PROGRAM ASSUMES THAT THE MATRIX ENTRIES ARE PROVIDED     LEC00250
C  EITHER COLUMN BY COLUMN OR ROW BY ROW.                         LEC00260
C  NOTE THAT THIS PROGRAM DOES NOT DIRECTLY APPLY TO THE         LEC00270
C  HERMITIAN CASE BECAUSE FOR HERMITIAN MATRICES THE DIAGONALS   LEC00280
C  ARE REAL AND THE OFF-DIAGONAL ENTRIES ARE COMPLEX VARIABLES.  LEC00290
C                                                    LEC00300
C  NONPORTABLE STATEMENTS:  PFORT VERIFIER INDICATES THAT THIS   LEC00310
C                           IS PORTABLE.                          LEC00320
C                                                    LEC00330
C-----LEC00340
C  DOUBLE PRECISION A(15000), AD(2000)                          LEC00350
C  DOUBLE PRECISION ZERO                                         LEC00360
C  INTEGER IROW(15000),ICOL(15000)                               LEC00370
C-----LEC00380
C  INPUT FILE 7 CONTAINS THE SPARSE SYMMETRIC NXN MATRIX STORED AS: LEC00390
C                                                    LEC00400
C           NZ,M,N,MATNO                                         LEC00410
C           I(K)  J(K)  A(K)  K = 1,NZ                            LEC00420
C                                                    LEC00430
C  WHERE NZ IS THE TOTAL NUMBER OF NONZEROS IN THE MATRIX A,    LEC00440
C  N IS THE ROW AND COLUMN DIMENSION OF A,                       LEC00450
C  AND A(K) ARE THE NONZERO ENTRIES STORED ROW BY ROW OR         LEC00460
C  COLUMN BY COLUMN.  PROGRAM READS THIS IN AS IROW(K) = I(K),  LEC00470
C  ICOL(K) = J(K), AND A(K) = A(K).                              LEC00480
C                                                    LEC00490
C  OUTPUT FILE = 8 CONTAINS THE A-MATRIX IN SPARSE FORMAT       LEC00500
C                                                    LEC00510
C           NZS,N,NZL,MATNO                                       LEC00520

```

```

C          ICOL(K)    K = 1,NZL          LEC00530
C          IROW(K)    K = 1,NZS          LEC00540
C          AD(K)      K = 1,N           LEC00550
C          A(K)       K = 1,NZS         LEC00560
C                                          LEC00570
C      WHERE N IS THE ORDER OF THE INPUT MATRIX A,          LEC00580
C      NZ EQUALS THE NUMBER OF NONZERO ELEMENTS IN A WHICH ARE ON LEC00590
C      OR BELOW THE MAIN DIAGONAL.  NZL EQUALS THE NUMBER OF THE LEC00600
C      LAST COLUMN HAVING NONZEROS BELOW THE DIAGONAL IN A. LEC00610
C      NZS EQUALS THE NUMBER OF NONZERO ELEMENTS BELOW THE MAIN LEC00620
C      DIAGONAL.  AD(K), K=1,N, CONTAINS THE DIAGONAL ELEMENTS OF A. LEC00630
C      A(K), K=1,NZS, CONTAINS THE KTH NONZERO SUB-DIAGONAL ELEMENT LEC00640
C      OF THE INPUT MATRIX.  A IS STORED COLUMN BY COLUMN. LEC00650
C      IROW(K), K=1,NZS, CONTAINS THE ROW INDEX OF THE NONZERO LEC00660
C      STRICTLY LOWER TRIANGULAR ELEMENT A(K). LEC00670
C      ICOL(K), K=1,NZL, EQUALS THE NUMBER OF STRICTLY LOWER LEC00680
C      TRIANGULAR NONZEROS IN COLUMN K OF THE INPUT MATRIX. LEC00690
C                                          LEC00700
C-----LECO0710
C      ZERO = 0.0D0          LEC00720
C                                          LEC00730
C      READ(7,10) NZ,N,MATNO,IROW LEC00740
10  FORMAT(2I6,I8,I4)      LEC00750
C                                          LEC00760
C      WRITE(6,20) NZ,N,MATNO,IROW LEC00770
20  FORMAT(I10,I6,I10,' = NO. NONZERO AIJ J.GE.I, ORDER OF A, MATNO'/ LEC00780
1  I6,' = IROW IF IROW=0 ORDERING IS BY COLS IROW=1 BY ROWS'/) LEC00790
C                                          LEC00800
C      DO 30 K = 1,N          LEC00810
30  AD(K) = ZERO            LEC00820
C                                          LEC00830
C      IF (IROW.EQ.0) READ(7,40) (IROW(K),ICOL(K),A(K), K=1,NZ) LEC00840
C                                          LEC00850
C      IF (IROW.EQ.1) READ(7,40) (ICOL(K),IROW(K),A(K), K=1,NZ) LEC00860
40  FORMAT(2I5,E14.7)      LEC00870
C                                          LEC00880
C      LCOUNT = 0          LEC00890
C      K = 1                LEC00900
C                                          LEC00910
C      START OF A NEW COLUMN LEC00920
50  CONTINUE                LEC00930
C      J = ICOL(K)          LEC00940
C      ICOL(J) = 0          LEC00950
60  CONTINUE                LEC00960
C                                          LEC00970
C      IF (J.NE.IROW(K)) GO TO 70 LEC00980
C                                          LEC00990
C      DIAGONAL CASE        LEC01000
C      AD(J) = A(K)         LEC01010
C      GO TO 80             LEC01020
C                                          LEC01030
C      SUB-DIAGONAL NONZERO LEC01040
70  CONTINUE                LEC01050
C      NZL = J              LEC01060
C      LCOUNT = LCOUNT + 1 LEC01070

```

	A(LCOUNT) = A(K)	LEC01080
	IROW(LCOUNT) = IROW(K)	LEC01090
	ICOL(J) = ICOL(J) + 1	LEC01100
C		LEC01110
	80 CONTINUE	LEC01120
	K = K+1	LEC01130
C		LEC01140
	IF(K.GT.NZ) GO TO 90	LEC01150
C		LEC01160
	IF(ICOL(K).GT.J) GO TO 50	LEC01170
C		LEC01180
	GO TO 60	LEC01190
C		LEC01200
	90 CONTINUE	LEC01210
	NZS = LCOUNT	LEC01220
C		LEC01230
	WRITE(8,100) NZS,N,NZL,MATNO	LEC01240
	WRITE(6,100) NZS,N,NZL,MATNO	LEC01250
	100 FORMAT(I10,2I6,I8,' = NZS N NZL MATNO')	LEC01260
C		LEC01270
	WRITE(8,110) (ICOL(I), I=1,NZL)	LEC01280
	WRITE(8,110) (IROW(K), K=1,NZS)	LEC01290
	110 FORMAT(13I6)	LEC01300
C		LEC01310
	WRITE(8,120) (AD(K), K=1,N)	LEC01320
	WRITE(8,120) (A(K), K=1,NZS)	LEC01330
	120 FORMAT(4E19.10)	LEC01340
C		LEC01350
C	-----END LCOMPAC-----	LEC01360
	STOP	LEC01370
	END	LEC01380

## 2.8 LEVAL: LEVEC: File Definitions, Sample Input Files

Below is a listing of the input/output files which are accessed by the real symmetric Lanczos eigenvalue program, LEVAL. Included also is a sample of the input file which LEVAL requires on file 5. The parameters are supplied in free format. LEVAL computes eigenvalues of real symmetric matrices  $A$  on user-specified intervals which must be supplied in ascending order. File 8 is assumed to contain the data which defines the real symmetric  $n \times n$  matrix  $A$ .

### Sample Specifications of the Input/Output Files for LEVAL

```
-----
LEVAL EXEC LANCZOS EIGENVALUE CALCULATION REAL SYMMETRIC MATRICES
FI 06 TERM
FILEDEF 1 DISK &1      NHISTORY  A (RECFM F LRECL 80 BLOCK 80
FILEDEF 2 DISK &1      HISTORY   A (RECFM F LRECL 80 BLOCK 80
FILEDEF 3 DISK &1      GOODEV   A (RECFM F LRECL 80 BLOCK 80
FILEDEF 4 DISK &1      ERRINV   A (RECFM F LRECL 80 BLOCK 80
FILEDEF 5 DISK LEVAL   INPUT    A (RECFM F LRECL 80 BLOCK 80
FILEDEF 8 DISK &1      INPUT    A (RECFM F LRECL 80 BLOCK 80
FILEDEF 11 DISK &1     DISTINCT A (RECFM F LRECL 80 BLOCK 80
LOAD  LEVAL  LESUB  LEMULT
-----
```

### Sample Input File for LEVAL

```
-----
LANCZOS EIGENVALUE COMPUTATIONS, NO REORTHOGONALIZATION
TEST MATRIX
LINE 1  N      KMAX      NMEVS      MATNO
      143      429          1      706830
LINE 2  SVSEED      RHSEED      MXINIT      MXSTUR
      7892713      147935          5      100000
LINE 3  ISTART      ISTOP
      0              1
LINE 4  IHIS      IDIST      IWRITE
      1              0          1
LINE 5  RELTOL (RELATIVE TOLERANCE IN 'COMBINING' GOODEV)
      .0000000001
LINE 6  MB(1)  MB(2)  MB(3)  MB(4) (ORDERS OF T(1,MEV))
      190
LINE 7  NINT      (NUMBER OF SUB-INTERVALS FOR BISEC)
      1
LINE 8  LB(1)  LB(2)  LB(3)  (INTERVAL LOWER BOUNDS)
      0.0
LINE 9  UB(1)  UB(2)  UB(3)  (INTERVAL UPPER BOUNDS)
      1.001
-----
```

Below is a listing of the input/output files which are accessed by the real symmetric Lanczos eigenvector program, LEVEC. Included also is a sample of the input file which LEVEC requires on file 5. The parameters are supplied in free format. LEVEC computes eigenvectors for each of a user-specified subset of the eigenvalues computed by the companion program LEVAL. Eigenvector approximations are computed only for eigenvalue approximations which have 'converged'.

#### Sample Specifications of the Input/Output Files for LEVEC

```
-----
LEVEC EXEC TO RUN LANCZOS EIGENVECTOR PROGRAM, REAL SYMMETRIC MATRICES
FI 06 TERM
FILEDEF 2 DISK &1      HISTORY  A (RECFM F LRECL 80 BLOCK 80
FILEDEF 3 DISK &1      GOODEV   A (RECFM F LRECL 80 BLOCK 80
FILEDEF 4 DISK &1      ERRINV   A (RECFM F LRECL 80 BLOCK 80
FILEDEF 5 DISK LEVEC   INPUT    A (RECFM F LRECL 80 BLOCK 80
FILEDEF 8 DISK &1      INPUT    A (RECFM F LRECL 80 BLOCK 80
FILEDEF 9 DISK &1      ERREST   A (RECFM F LRECL 80 BLOCK 80
FILEDEF 10 DISK &1     BOUNDS  A (RECFM F LRECL 80 BLOCK 80
FILEDEF 11 DISK &1     TEIGVECS A (RECFM F LRECL 80 BLOCK 80
FILEDEF 12 DISK &1     RITZVECS A (RECFM F LRECL 80 BLOCK 80
FILEDEF 13 DISK &1     PAIGE    A (RECFM F LRECL 80 BLOCK 80
LOAD LEVEC LESUB LEMULT
-----
```

#### Sample Input File for LEVEC

```
-----
LEVEC REAL SYMMETRIC EIGENVECTOR COMPUTATIONS, NO REORTHOGONALIZATION
LINE 1 MDIMTV MDIMRV MBETA (MAX.DIMENSIONS, TVEC, RITVEC AND BETA
      10000 10000 2000
LINE 2 RELTOL
      .0000000001
LINE 3 MBOUND NTVCON SVTVEC IREAD (FLAGS
      0 1 0 1
LINE 4 TVSTOP LVCONT ERCONT IWRITE (FLAGS
      0 1 1 1
LINE 5 RHSEED (RANDOM GENERATOR SEED FOR STARTING VECTOR IN INVERM
      45329517
LINE 6 MATNO N
      100 100
-----
```