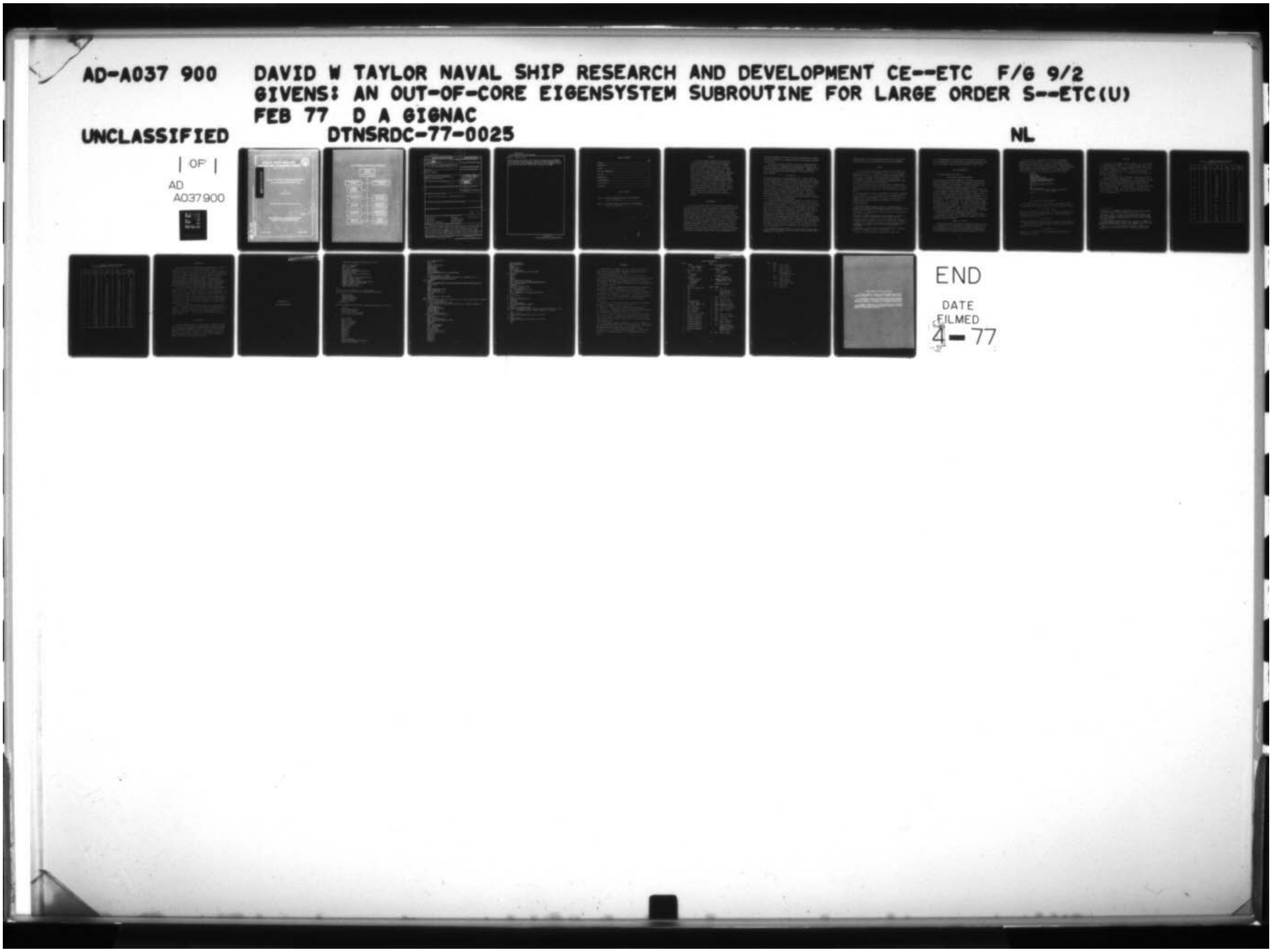

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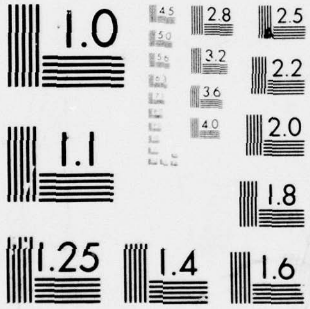

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GIVENS: AN OUT-OF-CORE EIGENSYSTEM SUBROUTINE FOR LARGE ORDER SYMMETRIC MATRICES

by

Donald A. Gignac

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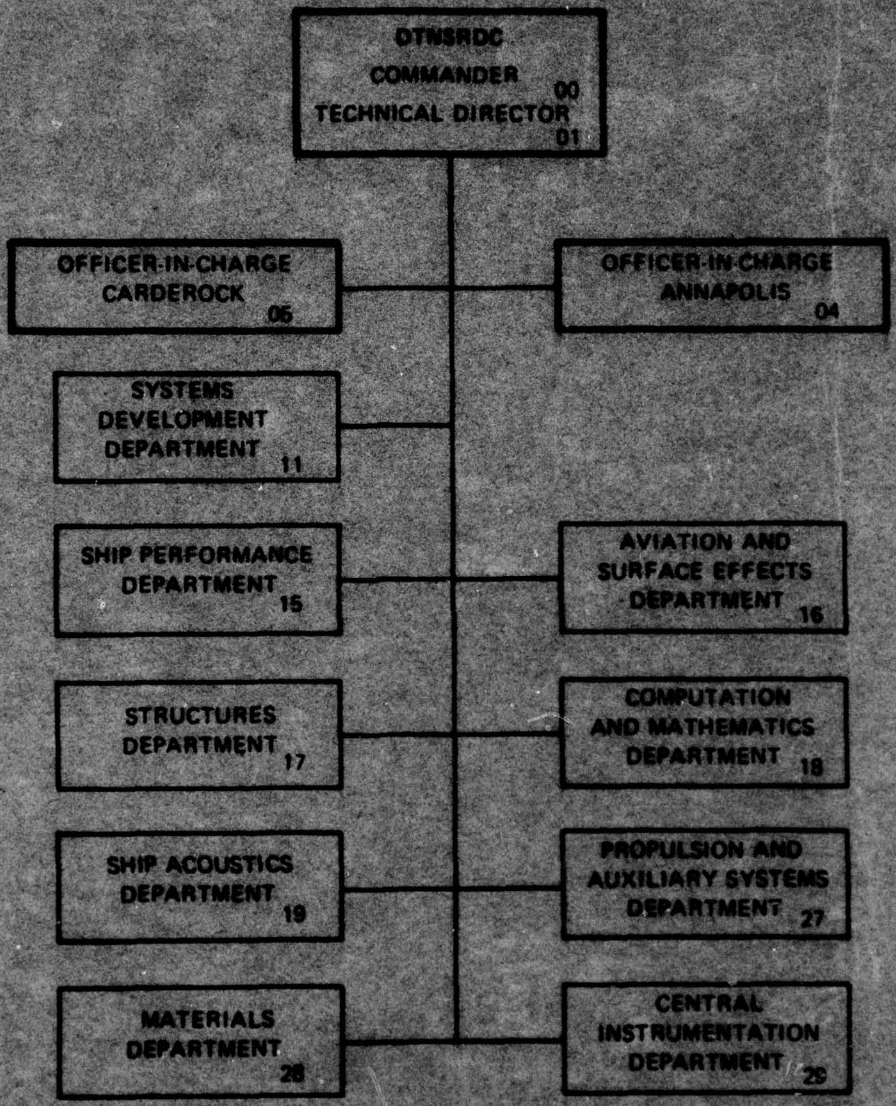

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The need to compute eigenvalues and eigenvectors for large order symmetric matrices arises frequently in the finite element approach to static structural analysis as well as in the applied work of many other fields in the Navy's varied research program. GIVENS is an out-of-core FORTRAN callable eigensystem subroutine which computes all the eigenvalues and specified eigenvectors for a large order real symmetric matrix using modifications of the GIVENS tridiagonalization procedure, the QR method of Francis, and inverse iteration.

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Item 20. Abstract (cont.)

GIVENS has been put together from subroutines extracted from the NASTRAN (NAsa STRuctural ANalysis) program. The use of GIVENS presupposes that the user can attach a special FORTRAN compiler and a certain subroutine library presently available on the CDC 6000 series computers at DTNSRDC.

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ABSTRACT

The need to compute eigenvalues and eigenvectors for large order symmetric matrices arises frequently in the finite element approach to static structural analysis as well as in the applied work of many other fields in the Navy's varied research program. GIVENS is an out-of-core FORTRAN callable eigensystem subroutine which computes all the eigenvalues and specified eigenvectors for a large order real symmetric matrix using modifications of the GIVENS tridiagonalization procedure, the QR method of Francis, and inverse iteration. GIVENS has been put together from subroutines extracted from the NASTRAN (NAsa STRuctural ANalysis) program. The use of GIVENS presupposes that the user can attach a special FORTRAN compiler and a certain subroutine library presently available on the CDC 6000 series computers at DTNSRDC.

INTRODUCTION

One of the long range projects of the Computation, Mathematics, and Logistics Department has been the development of mathematical subroutines suitable for use in the computer-aided structural analysis of ships. Many unrelated efforts in both government and industry have resulted in computer programs that treat particular classes of structural problems. These programs often involve the solution of similar mathematical problems but, since the solutions are reached independently, the efficiency and accuracy of the various algorithms used may vary greatly. The need to coordinate these diverse efforts, to develop improved methods of more general applicability, and to produce more comprehensive programs for solving Navy structural problems became obvious. A project was therefore established to coordinate research efforts involving mathematical and computational methods in the area of structural mechanics and to integrate the work of mathematicians, computer specialists, and structural engineers in this field.

The present considerable interest in the finite element approach to structural analysis is evidenced by the widespread use of NASTRAN (NAsa STRuctural ANalysis program)[1] and other such programs. Fundamental to the finite element approach to vibration analysis is the solution of the matrix equation

$$(K - \lambda M)U = 0$$

for natural frequencies (λ) and normal modes (U). If both K and M are real and symmetric and M is positive definite, this problem can be reduced to one of computing the eigensystem of a real symmetric matrix C. However, the order of the problem is often so large that, even when advantage is taken of sparsity, it is not feasible, and often not even possible, to store the matrix C in the core (high speed direct access) memory of a computer, let alone to compute C's eigensystem in core. The need to compute eigensystems for such large order real symmetric matrices also occurs quite frequently in the applied work of other scientific disciplines in the Navy's far-ranging research program.

The NASTRAN program has mathematical "modules" to cope with this and other mathematical or computational problems which arise in the course of the NASTRAN structural analysis. To be sure, these modules can be accessed directly for a mathematical problem as such but then DMI (Direct Matrix Input) cards are required for the matrices. Unfortunately, this DMI card procedure is not realistic for large order matrices. Accordingly, an investigation was undertaken to see whether some of the mathematical capabilities of these modules could be extracted from the NASTRAN program and recast in the form of FORTRAN callable subroutines with a more efficient input facility for large order matrices. The present GIVENS subroutine was put together in this way with the assistance of Mr. Myles Hurwitz (Code 1844) who removed the appropriate subroutines from the NASTRAN READ (Real

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[1] "The NASTRAN User's Manual (Level 15.0)," NASA SP-222, Scientific and Technical Information Office, National Aeronautics and Space Administration, Washington, D.C., June 1972.

Eigenvalue Analysis for the Displacement method) module along with the required general library input and output subroutines from NASTRAN.

THEORY

This section briefly describes the procedure used by GIVENS to compute the eigensystem of a real symmetric matrix. For a more detailed presentation the reader is referred to the NASTRAN Theoretical Manual[2] or to the authors cited below. The GIVENS procedure is as follows:

(1) The matrix is reduced to a real symmetric tridiagonal matrix using Wilkinson's modification[3] of the GIVENS method.[4]

(2) All the eigenvalues of this tridiagonal matrix are computed using Ortega and Kaiser's modification[5] of the QR method of Francis.[6] Since the two matrices are similar, these are also the eigenvalues of the original matrix.

(3) Certain eigenvectors (those corresponding to the smallest eigenvalues of those eigenvalues in a certain range) of the tridiagonal matrix are computed using a method developed by Wilkinson.[7] The Gram-Schmidt algorithm[8] is used to insure eigenvector orthonormality in the case of repeated eigenvalues.

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[2] "The NASTRAN Theoretical Manual (Level 15.0)," NASA SP-221(01), Scientific and Technical Information Office, National Aeronautics and Space Administration, Washington, D.C., December 1972, pp. 10.1-1, 10.2-15.

[3] Wilkinson, J.H., "The Algebraic Eigenvalue Problem," Oxford University Press, 1965, pp. 506-510.

[4] Givens, W., "Numerical Computation of the Characteristic Values of a Real Symmetric Matrix," Oak Ridge National Lab., ORNL-1574, 1954.

[5] Ortega, J.M. and H.F. Kaiser, "The LL^T and QR Methods for Symmetric Tridiagonal Matrices," Computer J., Vol. 6, No. 1 (Jan. 1963), pp. 99-101.

[6] Francis, J.G.F., "The QR Transformation, a Unitary Analogue to the LR Transformation," Computer J., Vol. 4, No. 3 (Oct. 1961) and No. 4 (Jan. 1962).

[7] Wilkinson, J.H., "The Calculation of the Eigenvectors of Codiagonal Matrices," The Computer J., Vol. 1, 1958, pp. 90.

[8] Bodewig, E., "Matrix Calculus," Interscience Publisher, 1959.

(4) The eigenvectors of the original matrix are obtained from those of the tridiagonal matrix by multiplying each tridiagonal eigenvector by the series of orthogonal rotation matrices determined by GIVENS' method.[2]

THE GIVENS SUBROUTINE

The calling sequence for GIVENS is

CALL GIVENS(N,NV,JTIME,LFREC,HFREC)

The value of the first integer argument N is the order n of the matrix. Now n must be entered as the value of some variable N rather than as a numerical constant, since the argument N is redefined in GIVENS. This restriction does not apply to the other arguments of GIVENS.

The values of the second integer parameter NV and of the fourth and fifth real arguments LFREC and HFREC are assigned as follows: If the user wishes to compute the eigenvectors of the k smallest eigenvalues, the value of NV is k and the values of LFREC and HFREC are immaterial. If the user wishes to compute the eigenvectors corresponding to eigenvalues λ in the interval $a < \lambda < b$, the value of NV is zero and the values of LFREC and HFREC are a and b, respectively. The number of eigenvectors computed is returned through the argument NV. If the user merely wishes all the eigenvalues and no eigenvectors, the value of NV is zero and the common value of LFREC and HFREC is c, where c is not an eigenvalue. (The reader is reminded that GIVENS always computes all the eigenvalues.)

The value of the third integer argument JTIME is a time estimate (integral number of seconds) for the eigensystem computation. One such estimate is given by the formula

$$\mathrm{JTIME} = N^3 + 15\mathrm{x}10^{-5} .$$

GIVENS reads the rows (or columns) of the matrix from tape 8, a row (or a column) at a time. GIVENS writes the eigensystem output on tape 9 in the following way. The first record contains the N eigenvalues and the succeeding NV records contain the specified eigenvectors (if any).

At present GIVENS is available in the form of a pre-compiled permanent file on the CDC 6400. The user's calling program must be compiled with the FORTRAN compiler originally used to compile NASTRAN to ensure compatibility with certain NASTRAN subroutines. GIVENS also requires certain subroutines from the SYSMISC library. The sample setup below illustrates the control cards required for GIVENS on the CDC 6400.

```
JOB CARD
CHARGE CARD
ATTACH,SYSMISC
LIBRARY,SYSMISC,SYSIO.
ATTACH,FILE,GIVENSEIGNSYM,ID=CAD6.
ATTACH,FTN,FTN3POLV340,ID=CSYS.
FTN CARD
RFL (to field length on job card)
LOAD,FILE.
LGO.
END OF RECORD CARD
PROGRAM MAIN(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,
                             TAPE8, TAPE9)
REAL LFREC
   .
   .
   N =
   .
   .
CALL GIVENS(N,NV,JTIME,LFREC,HFREC)
```

The field length CM for the job card may be determined as follows: CM_6, the amount of core memory required by GIVENS, is given by the formula

$$CM_6 = N^2 + 6N + 2655_{10}$$

where CM_6 is expressed as an octal number. Let CM_M be an estimate for the field length of the calling program for GIVENS. Then the total field length CM is the octal sum

$$CM = CM_M + CM_6$$

(CM_M can be determined more exactly from the load map of a successful run.)

Similarly the time T (integral number of seconds) for the job card is obtained from the decimal sum

$$T = T_M + JTIME$$

where T_M is a time estimate for the calling program and JTIME is the third argument of GIVENS.

THE TESTS

Let A_n be the real symmetric matrix of order n = 10, 120, 10 with 10 on the diagonal and 1 elsewhere. A_n is a positive definite matrix with n-1 repeated eigenvalues of 9 and one eigenvalue of 9+n.[9] Let B_n be the real symmetric banded matrix of order n = 10, 120, 10 obtained by imposing a bandwidth of 10 on A_n. B_n is likewise positive definite but with distinct eigenvalues.

Table 1 contains the times (in seconds) for tridiagonalization and the tridiagonal eigenvalue computation for A_n. Table 2 contains the same data for B_n. Four subroutine implementations of the basic algorithm outlined previously are compared in these tables: GIVENS; TRI4 and IMQL2;[10] EHOUSS and EQRT25;[11] TRED1 and IMTQL1.[12] The times were obtained on the CDC 6400 at DTNSRDC. The GIVENS times were obtained with the Scope 3.3 operating system, and the other times were obtained with the Scope 3.4 operating system.

---

[9] Westlake, J., "A Handbook of Numerical Matrix Inversion and Solution of Linear Equations," John Wiley & Sons, Inc., 1968, p. 141.

[10] Nikolai, P.J. and N.-K. Tsao, "The ARL LINEAR ALGEBRA LIBRARY Handbook," Interim Report, 1 September 1973-31 March 1974, ARL TR 74-0106 (July 1974), Aerospace Research Laboratories, Air Force Systems Command, Wright-Patterson AFB.

[11] The IMSL LIBRARY 3 Reference Manual, Vol. I, Edition 4 (FORTRAN 2.4) CDC 6200/6400/6500/6600/7600 (1975), revised November 1974, International Mathematical and Statistical Libraries, Inc., Houston, Texas.

[12] Smith, B.T., et al, "Matrix Eigensystem Routines - EISPACK Guide," Lecture notes in Computer Science, Vol. 6, Springer-Verlag, New York (1974).

TABLE 1 - EIGENVALUE COMPUTATION TIMES FOR A FULL MATRIX A_N (N = 10, 120, 10)

N	GIVENS	ARL	IMSL	EISPACK
10	.138	0.	+.008	.019
	.16	0.	.018	0.
20	.380	.25	.107	0.
	.33	.619	.019	0.
30	.797	.781	.371	.441
	.45	.0231	.019	0.
40	1.543	.254	.793	.904
	.63	.0110	.056	0.
50	2.675	3.444	1.515	1.603
	.89	+.019	.039	.201
60	4.276	.307	2.547	2.51
	.115	+.003	+.079	.638
70	6.4	9.186	3.998	3.869
	.145	0.	+.078	.654
80	9.137	.539	5.919	5.629
	.181	0.	.12	.698
90	12.582	18.72	8.302	7.934
	.222	+.02	.116	1.103
100	16.766	.819	11.297	10.6350
	.263	0.	.136	2.001
110	21.901	33.473	14.91	14.178
	.313	+.02	.192	2.726
120	27.856	43.869	19.299	18.078
	.360	+.043	.213	3.326

TABLE 2 - EIGENVALUE COMPUTATION TIMES FOR A 10-BANDED MATRIX B_N (N = 10, 120, 10)

N	GIVENS	ARL	IMSL	EISPACK
10	.131	0.	.031	0.
	.022	0.	0.	0.
20	.332	.25	.116	.116
	.280	0.	.105	.129
30	.722	.727	.359	.365
	.319	.199	.122	.167
40	1.308	1.819	.804	.772
	1.050	.452	.401	.508
50	2.249	3.421	1.533	1.44
	1.211	.654	.421	.566
60	3.501	5.692	2.587	2.439
	2.124	1.106	.775	1.046
70	5.287	9.07	4.04	3.581
	2.516	1.159	.935	1.164
80	7.645	13.116	5.896	5.392
	3.379	1.386	1.169	1.629
90	10.519	18.464	8.374	7.749
	4.337	2.161	1.584	2.114
100	14.033	25.082	11.270	10.299
	5.560	2.617	2.036	2.752
110	18.328	33.138	14.949	13.625
	6.608	3.374	2.443	3.266
120	23.601	42.781	19.237	17.722
	7.591	3.78	2.78	3.731

OBSERVATIONS

The GIVENS program was undertaken with a twofold purpose: first, to see how difficult it is to extract a NASTRAN module, recast it as a stand-alone FORTRAN callable subroutine, and then evaluate this subroutine as such; and second, to provide an out-of-core eigensystem capability for users of our computer. This work has indicated that it is not too difficult to remove a NASTRAN module and make a subroutine out of it -- assuming familiarity with the NASTRAN program. In the present instance the NASTRAN expertise was provided by Mr. Myles Hurwitz of Code 1844. Module removal should not be attempted without a NASTRAN consultant.

No out-of-core symmetric matrix eigensystem solvers were at hand to compare with GIVENS. Accordingly, suitable in-core subroutines were chosen from the various subroutine libraries for comparison purposes. The times for these comparison runs are presented in Tables 1 and 2. All four subroutines produced virtually identical results as regards accuracy. It should also be borne in mind that GIVENS requires significant amounts of "PP" time. The behavior of the ARL subroutine TRI4 is surprising and warrants investigation.

GIVENS is an experimental program. Because it was extracted from NASTRAN, it is perhaps a bit more complicated than if it had been written directly. As expected, GIVENS has a time disadvantage when in-core computation is possible. GIVENS is meant for sparse matrices too large to fit in core.

ACKNOWLEDGMENTS

The author wishes to thank Dr. Elizabeth Cuthill (DTNSRDC Code 1805) for her interest and advice and to acknowledge the invaluable assistance of Mr. Myles Hurwitz (DTNSRDC Code 1844) in putting the GIVENS program together. He also wishes to thank the following people for their help: Mr. Michael Golden (DTNSRDC Code 1844); Mrs. Nora Taylor (DTNSRDC Code 1890); and Mrs. Sharon Good (DTNSRDC Code 1892).

GIVENS LISTING

(see following pages)

```
      SUBROUTINE GIVENS(N,NV,JTIME,LFREC,HFREC)
C
      INTEGER T,T1,T2,T3
      INTEGER SYSBUF
      REAL LFREC
      EXTERNAL READ,WRITE
      DIMENSION MCB(7),IZ(1),IITLE(1)
      DIMENSION NAM(2)
      EQUIVALENCE (Z,IZ),(TITLE,IITLE)
      COMMON Z(1)
      COMMON /PACKX/ IN,IOUT,II,NN,INCR
      COMMON /GIVN/ TITLE(150)
      COMMON /STIME/ ITIME
      COMMON /UNPAKX/ ITOUT,III,NNN,IINCR
      COMMON /SYSTEM/ SYSBUF,NOUT
      COMMON /MSGX/ NMSG
      DATA NAM/4HGIVE,4HNS  /
C
C
C SET UP END OF OPEN CORE FOR GINO INDICES
C NFILES=(NO. OF GINO FILES+1)*(NBRMST+1)=21*63=1323
C
      NFILES=1323
      LCORE=KORSZ(Z)
      LCORE=LCORE+NFILES
      J=LCORE-NFILES+1
      DO 28 K=J,LCORE
   28 IZ(K)=0
C
C SET UP ADDRESS 76B FOR THOSE ROUTINES USING CORSZ, NOT KORSZ
C
      LCORE=0
      CALL FIELDLN(LCORE)
      LCORE=LCORE-NFILES
      CALL XSTORE(LCORE,1,76B)
      CALL XSTORE(LCORE,1,63B)
C
C
      ITIME=JTIME
    4 IITLE(101)=N
      TITLE(102)=LFREC
      TITLE(105)=HFREC
      IITLE(107)=NV
      TITLE(110)=0
      MCB(1)=304
      MCB(2)=0
      MCB(3)=N
      MCB(4)=6
      MCB(5)=1
      MCB(6)=0
      MCB(7)=0
      NN=N
      LLCORE=KORSZ(Z)
      ISTORE=MAX0(19*N,7*N+2*SYSBUF)
      IMORE=ISTORE-LLCORE
```

```
      IF (IMORE)27,27,30
   27 NZ=LLCORE
      AN=N
      AZ=NZ-6*N-2*SYSBUF
      AM=SQRT(AZ)
      AK=AN-AM+1.
      AMB=15.E-6
      APAK=140.E-6
      T1=9.0*AN*AN*AN*AMB+11.0*AN*AN*APAK
      T2=0.0
      IF (AK.LE.0.0) GO TO 1101
      T2=APAK*(AK*(AK+1.0)*(AN+2.0)-(AN+AN+3.0)*AK*(AK+1.0)*.5
     1    +AK*(AK+1.0)*(AK+AK+1.0)/6.0)
 1101 CONTINUE
      AV=NV
      T3=6.0*AN*AN*AV*AMB+3.0*AV*AV*AN*AMB+6.*AV*AN*APAK+AV*AV*APAK
      T=T1+T2+T3
      N=AN
      M=AM
      WRITE(NOUT,1000)T,N,M
      CALL TMTOGO(I)
      IF(I.GE.T) GO TO 101
      IP1=-50
      IFILE=T
      CALL MESAGE(IP1,IFILE,NAM)
  101 CONTINUE
 1000 FORMAT(60H0*** USER INFORMATION MESSAGE 2016, GIVENS TIME ESTIMATE
     * IS ,I8, 9H SECONDS. /
     * 36X,16HPROBLEM SIZE IS ,I8,
     *    54H, SPILL WILL OCCUR FOR THIS CORE AT A PROBLEM SIZE OF ,
     *  I8,2H .)
      LCORE=KORSZ(Z)
      IBUF=LCORE-SYSBUF+1
      LCORE=IBUF-1
      IMORE=N-LCORE
      IF (N-LCORE)29,29,30
   29 CALL GOPEN(304,Z(IBUF),1)
      REWIND 8
      DO 5 J=1,N
      READ( 8) (Z(I),I=1,N)
      CALL PACK(Z(1),304,WRITE,MCB)
    5 CONTINUE
      REWIND 8
      CALL CLOSE(304,1)
      CALL WRTTRL(MCB)
      CALL VALVEC
      NV=IITLE(107)
      IF (NV.LE.1) GO TO 62
      IF(N.EQ.1)GO TO 62
      MCB(1)=203
      MCB(2)=N
      MCB(3)=N
      MCB(4)=8
      MCB(5)=2
      MCB(6)=2
```

```
      MCB(7)=10000./N
      CALL WRTTRL(MCB)
      MAA=203
      EPSII=1.E-4
      MCB(1)=305
      CALL RDTRL(MCB)
      CALL READ4(201,MCB,306,EPSII,MAA)
   62 CONTINUE
      ITOUT=1
      III=1
      NNN=N
      IINCR=1
      CALL GOPEN(201,Z(IBUF),0)
      CALL READ(201,Z(1),N,0,M),RETURNS(40,45)
      CALL CLOSE(201,1)
      REWIND 9
      WRITE(9)(Z(LK),LK=1,N)
      IF (NV) 34,35,34
   34 CALL GOPEN(305,Z(IBUF),0)
      DO 10 J=1,NV
      CALL UNPACK(305,Z(1),READ),RETURNS(15)
      GO TO 25
   15 DO 20 I=1,N
   20 Z(I)=0.
   25 WRITE(9)(Z(LK),LK=1,N)
   10 CONTINUE
      REWIND 9
      CALL CLOSE(305,1)
   35 IF (NMSG.GT.0) CALL MSGWRT
      RETURN
   30 WRITE( 6,31)IMORE,IMORE
   31 FORMAT(1H1/14(1H0/)/37X,13HINSUFFICIENT CORE.,I8,3H / ,O8,
     1        41H MORE DECIMAL / OCTAL LOCATIONS REQUIRED.)
      STOP
   40 WRITE( 6,41)
   41 FORMAT(1H1/14(1H0/)/61X,12HEOF ON LAMA.)
      STOP
   45 WRITE( 6,46)
   46 FORMAT(1H1/14(1H0/)/61X,12HEOR ON LAMA.)
      STOP
      END
```

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