Yale Sparse Matrix Package
I. The Symmetric Codes
S. C./Eisenstat, M. C./Gursky, M. H./Schultz, A. H./Sherman
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Department of Computer Science, Yale University.

Department of Electrical Engineering and Computer Science, University of California, Berkeley.

Department of Computer Sciences, The University of Texas at Austin.
1. Introduction

Consider the $N \times N$ system of linear equations

\[(1) \quad Mx = b,\]

where the coefficient matrix $M$ is large, sparse, symmetric, and positive definite. Such systems arise frequently in scientific computation, e.g., in finite difference and finite element approximations to elliptic boundary value problems. In this report, we present a package of efficient, reliable, well-documented, and portable FORTRAN subroutines for solving these systems.

Direct methods for solving (1) are generally variations of symmetric Gaussian elimination. We form the $U^T D U$ decomposition of $A$, where $U$ is unit upper triangular and $D$ positive diagonal, and then successively solve the triangular systems

\[(2) \quad U^T y = b, \quad Dz = y, \quad Ux = z.\]

When $M$ is large ($N \gg 1$), (dense) Gaussian elimination is prohibitively expensive in terms of both the work ($\sim 1/3 N^3$ multiplies) and storage ($N^2$ words) required. But, since $M$ is sparse, most entries of $M$ and $U$ are zero and there are significant advantages to factoring $M$ without storing or operating on the zeroes appearing in $M$ and $U$. Recently, a number of implementations of sparse Gaussian elimination have appeared based on this idea, cf. [2,5,6,7].

In section 2, we describe the scheme used for storing sparse matrices, while in Section 3 we give an overview of the package from the point of view of the user; for further details of the algorithms employed, see [4,9]. In section 4, we illustrate the performance of the
package on a typical model problem. Listings of the ordering
subroutines and the subroutines for factoring and solving sparse
symmetric positive definite systems appear as Appendices 1 and 2.
Appendix 3 contains a test driver, a sample output of which appears as
Appendix 4.
2. **A Sparse Matrix Storage Scheme**

Since the coefficient matrix $M$ and the upper triangular factor $U$ are large and sparse, it is inefficient to store them as dense matrices. Instead, we store matrices using a row-by-row storage scheme used in previous implementations of sparse symmetric Gaussian elimination, cf. [1,4].

This scheme requires three one-dimensional arrays: $IA$, $JA$, and $A$. The nonzero entries of $M$ are stored row-by-row in the REAL array $A$. To identify the individual nonzero entries in a row, we need to know in which column each entry lies. The INTEGER array $JA$ contains the column indices which correspond to the nonzero entries of $M$, i.e., if $A(K) = M(I,J)$, then $JA(K) = J$. In addition, we need to know where each row starts and how long it is. The INTEGER array $IA$ contains the indices in $JA$ and $A$ where each row of $M$ begins, i.e., if $M(I,J)$ is the first (leftmost) entry of the $I^{th}$ row and $A(K) = M(I,J)$, then $IA(I) = K$. Moreover, $IA(N+1)$ is defined as the index in $JA$ and $A$ of the first location following the last element in the last row. Thus, the number of entries in the $I^{th}$ row is given by $IA(I+1) - IA(I)$, and the nonzero entries of the $I^{th}$ row are stored consecutively in $A(IA(I))$, $A(IA(I)+1)$, $\ldots$, $A(IA(I+1)-1)$ and the corresponding column indices are stored consecutively in $JA(IA(I))$, $JA(IA(I)+1)$, $\ldots$, $JA(IA(I+1)-1)$. 
For example, the 5x5 matrix
\[
M = \begin{bmatrix}
1 & 0 & 2 & 3 & 0 \\
0 & 4 & 0 & 0 & 0 \\
2 & 0 & 5 & 6 & 0 \\
3 & 0 & 6 & 7 & 8 \\
0 & 0 & 0 & 8 & 9
\end{bmatrix}
\]
is stored as
\[
\begin{array}{cccccccccccc}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 \\
\hline
\end{array}
\]
\[
\begin{array}{c}
IA \\
JA \\
A
\end{array}
\begin{array}{cccccccccccc}
1 & 4 & 5 & 8 & 12 & 13 \\
1 & 3 & 4 & 2 & 1 & 3 & 4 & 1 & 3 & 4 & 5 & 5 \\
1 & 2 & 3 & 4 & 2 & 5 & 6 & 3 & 6 & 7 & 8 & 9
\end{array}
\]

Since the matrix M is symmetric, it suffices to store only the nonzero entries in the diagonal and strict upper triangle of M. The storage scheme used is the same as before (except that nonzero entries in the strict lower triangle of M are ignored), and our example matrix would be stored as
\[
\begin{array}{cccccccccccc}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\hline
\end{array}
\]
\[
\begin{array}{c}
IA \\
JA \\
A
\end{array}
\begin{array}{cccccccccccc}
1 & 4 & 5 & 7 & 9 & 10 \\
1 & 3 & 4 & 2 & 3 & 4 & 4 & 5 & 5 \\
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9
\end{array}
\]

The overhead in this storage scheme is the storage required for the INTEGER arrays IA and JA. But since IA has \(N+1\) entries and JA has one entry for each element of A, the total overhead is approximately equal
to the number of nonzero entries in (the diagonal and strict upper triangle of) M.
3. A Sparse Symmetric Matrix Package

The package consists of three drivers and five subroutines (see Figure 1). The ordering driver (subroutine ODRV) may be used to symmetrically reorder the variables and equations so as to reduce the total work (i.e. the number of multiplies) and storage required. The solution driver (subroutine SDRV) is used to solve the (permuted) system of linear equations. The test driver (program STST) sets up a model sparse symmetric positive definite system of linear equations, calls ODRV to reorder the variables and equations, and calls SDRV to solve the linear system. In the remainder of this section, we describe each of these routines in somewhat greater detail. The codes themselves are extensively documented; for further details about the algorithms employed, see [4,9].

Figure 1: A schematic overview of the sparse symmetric matrix package
A. The Ordering Driver (ODRV)

The work and storage required to solve a large sparse system of linear equations clearly depend upon the zero-nonzero structure of the coefficient matrix. But since this matrix is symmetric and positive definite, we could equally well solve the permuted system

\[ Q M Q^T y = Q b, \quad Q x = y \]

given any permutation matrix \( Q \). The permuted system corresponds to symmetrically reordering the variables and equations of the original system, and the net result can often be a significant reduction in the work and storage required to form the \( U^T D U \) decomposition of \( A \) [3].

The ordering driver (subroutine ODRV) uses the important heuristic, the minimum degree algorithm (implemented in subroutine ORDER), to select \( Q \). ORDER does a symbolic elimination on the nonzero structure of the system. At each step, it chooses a pivot element from among those uneliminated diagonal matrix entries which require the fewest arithmetic operations to eliminate (ties are broken arbitrarily). This has the effect of locally optimizing the elimination process with respect to the number of arithmetic operations performed. See [8,9] for more details.

ORDER returns two one-dimensional INTEGER arrays of length \( N \): \( P \) contains the permutation of the row and column indices of \( M \), i.e., the sequence of pivots; and \( IP \) contains the inverse permutation, i.e., \( IP(P(I)) = I \) for \( I = 1, 2, \ldots, N \). If only the upper triangle of \( M \) is being stored, then the representation of \( M \) (i.e., the arrays \( IA \), \( JA \), and \( A \)) must be rearranged using the subroutine SRO (PATH=2 in ODRV).
The user may bypass ODRV entirely by setting \( P(I) = IP(I) = 1 \)
for \( I = 1, 2, 3, \ldots, N \). Alternately, the user may substitute another
ordering subroutine for ORDER, as long as it produces the two
permutations \( P \) and \( IP \). But again, if only the upper triangle of \( M \) is
being stored, the representation of \( M \) must be rearranged using SRO.

B. The Solution Driver (SDRV)

The solution driver (subroutine SDRV) is used to solve the
(permutated) linear system. Following Chang [1], SDRV breaks the solution
process into three steps: symbolic factorization (subroutine SSF),
numerical factorization (subroutine SNF), and back-solution (subroutine
SNS). First, SSF determines the nonzero structure of the rows of \( U \) from
the nonzero structure of the rows of \( M \). Second, SNF uses the structure
information generated by SSF to compute the \( U^tDU \) factorization of \( M \).
Third, SNS computes the solution \( x \) from the factorization generated by
SNF and the right-hand side \( b \).

By splitting up the computation, we have gained flexibility. To
solve a single system of equations, it suffices to use SSF, SNF, and SNS
(PATH=1 in SDRV). To solve several systems in which the coefficient
matrices have the same nonzero structure, it suffices to use SSF only
once and then to use SNF and SNS for each system (PATH=2). To solve
several systems with the same coefficient matrix but different right
hand sides, it suffices to use SSF and SNF only once and then use SNS
for each system (PATH=3).
C. The Test Driver (STST)

The test driver (program STST) is used to verify the performance of the package on a particular computer system, and may be used as a guide to understanding how to use the package. It generates the coefficient matrix for the standard five-point finite difference approximation on a 3x3 grid to the Poisson equation and chooses the right-hand side so that the solution vector $x$ is $(1, 2, 3, 4, 5, 6, 7, 8, 9)$. Since $M$ is symmetric, we can specify either the entire matrix (CASE=1) or only the upper triangle (CASE=2). STST then calls ODRV to reorder the variables and equations, and SDRV to solve the linear system. At each stage, the values of all relevant variables are printed out. A sample output appears as Appendix 4.
4. **Performance**

One of the most important aspects of any package is its performance in terms of both the time and storage required to solve a typical problem. In Tables I and II, we present the time and storage required to solve the familiar five-point finite difference equations on an $n \times n$ grid for several values of $n$. These computations were performed in single precision on an IBM 370/158 using the FORTRAN X optimizing compiler.

**Table I**

**Time Required**

Five-Point Operator on an $n \times n$ Grid

<table>
<thead>
<tr>
<th>Grid</th>
<th>STST</th>
<th>ORDER</th>
<th>SRO</th>
<th>SSF</th>
<th>SNF</th>
<th>sec/*</th>
<th>SNS</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.083</td>
<td>0.657</td>
<td>0.043</td>
<td>0.100</td>
<td>0.407</td>
<td>14.016</td>
<td>0.087</td>
<td>0.593</td>
</tr>
<tr>
<td>30</td>
<td>0.190</td>
<td>1.750</td>
<td>0.100</td>
<td>0.257</td>
<td>1.430</td>
<td>13.002</td>
<td>0.230</td>
<td>1.917</td>
</tr>
<tr>
<td>40</td>
<td>0.340</td>
<td>3.656</td>
<td>0.177</td>
<td>0.503</td>
<td>3.700</td>
<td>12.449</td>
<td>0.470</td>
<td>4.673</td>
</tr>
</tbody>
</table>
Table II

Storage Required

Five-Point Operator on an n x n Grid

<table>
<thead>
<tr>
<th>Grid</th>
<th>A, JA</th>
<th>U</th>
<th>JU</th>
<th>Total</th>
<th>Mults.</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1,160</td>
<td>3,368</td>
<td>1,889</td>
<td>7,259</td>
<td>35,195</td>
</tr>
<tr>
<td>30</td>
<td>2,640</td>
<td>9,456</td>
<td>4,538</td>
<td>18,496</td>
<td>127,666</td>
</tr>
<tr>
<td>40</td>
<td>4,720</td>
<td>19,926</td>
<td>8,423</td>
<td>36,351</td>
<td>334,937</td>
</tr>
</tbody>
</table>
5. References


Appendix I

Sparse Matrix Reordering Routines

*** Subroutine ODRV
*** Driver for sparse matrix reordering routines

SUBROUTINE ODRV
* (N, IA, JA, A, P, IP, NSP, ISP, PATH, FLAG)

PARAMETERS
Class abbreviations:
V - supplies a VALUE to the driver
R - contains a RESULT returned by the driver
I - is used INTERNALLY by the driver
A - is an ARRAY
N - is an INTEGER variable
F - is a REAL variable.

Class | Parameter
-------
| ------
V | The nonzero entries of the matrix M are stored row by row in the array A. The array JA contains the corresponding column indices; i.e. if A(K) = M(I,J), then JA(K) = J. The array IA contains pointers to delimit the rows of M; IA(I) is the index in JA and A of the first entry stored in the Ith row of M. For example, the symmetric 5 by 5 matrix
| 1 0 2 3 0
| 0 4 0 0 0
| 2 0 5 6 0
| 3 0 6 7 8
| 0 0 0 8 9
| would be stored as
| IA | 1 4 5 7 9 10
| JA | 1 3 4 2 3 4 4 5 5
| A | 1 2 3 4 5 6 7 8 9
| IA(I+1) - IA(I) is the number of nonzero entries in row I, so IA(N+1), where N is the number of rows in M, is needed to determine the length of the Nth row in A.
| If M is a symmetric matrix only the elements of the upper triangle (including the diagonal) need be stored in A, although the full matrix may be stored.

Vn | N - the number of rows/columns in matrix M.
Vfa | A - coefficient matrix for the system of linear equations
| Mx = b, stored in compressed form.
| Size = number of nonzeros in M (or only in upper triangle of M for symmetric matrix).
Vna | IA - pointers to first elements of each row in A.
| Size = N+1.
Vna | JA - the column numbers corresponding to elements of A.
| Size = size of A.
A minimum degree ordering of the matrix is done (ORDER). If
M is symmetric and only the upper triangle is being stored, the
array A needs to be reordered.

PATH - information on which subroutines are to be called.

Values and meanings of PATH are:

1. perform minimum degree ordering only.
2. perform minimum degree ordering and
   reordering of symmetric matrix. This
   value should be passed only if M is
   symmetric and only the nonzeros of the
   upper triangle of M are being
   stored. If the nonzeros of the entire
   matrix are being stored, PATH should
   equal 1.

FLAG - flag for error return from subroutines. Error values
and their meanings are:

0. no error
N+i. null row in A -- I
9N+i. ORDER storage exceeded on row I
10N+i. ISP too small to allocate space
11N+i. PATH out of bounds

The result of the ordering algorithm is a permutation of the
row numbers of M and the inverse of the permutation. The order
of the columns is the same as for the rows.

IP - inverse of the ordering of the rows/columns of M.
Size = N.
P - ordering of the rows/columns of M.
Size = N.

Workspace is needed to hold the temporary vectors used in the
ordering routine.

NSP - dimensioned size of ISP. NSP must generally be at
least 2*(number of pairs (I,J) such that M(I,J)
or M(J,I) is nonzero) + N for the ordering routine
and at least N + size of A for the symmetric
reordering routine.
ISP - storage space divided up for various arrays of
the subroutines.

INTEGER IA(1), JA(1), P(1), IP(1), PATH, FLAG, VV, TMP, Q
REAL A(1), ISP(1)

IF (PATH.LT.1 .OR. PATH.GT.2) GO TO 111

Allocate space for ordering subroutine ************************
MAX = NSP/2
VV = 1
LV = VV + MAX
IF (MAX.LT.N) GO TO 110

Call minimum degree ordering routine ************************
FLAG = 0
CALL ORDER
* (N, IA, JA, P, IP, MAX, ISP(VV), ISP(LV), FLAG)
IF (FLAG.NE.0) GO TO 100
C***** Allocate space, call symmetric reorder routine **************
IF (PATH.LT.2) GO TO 1
   TMP = 1
   Q = TMP + N
   IF (NSP+I-Q .LT. IA(N+I)-1) GO TO 110
   CALL SRO
   * (N, IP, IA, JA, A, ISP(TMP), ISP(Q))
1  RETURN
C
C** ERROR: Error Detected in ORDER
100  RETURN
C** ERROR: Insufficient Storage
110  FLAG = 10*N + 1
     RETURN
C** ERROR: Illegal PATH Specified
111  FLAG = 11*N + 1
     RETURN
END
C
C
C*** Subroutine ORDER
C*** Minimum degree ordering algorithm with threshold search
C
SUBROUTINE ORDER
   * (N, IA, JA, P, IP, MAX, VV, LV, FLAG)
       C
C       Input variables: N, IA, JA, MAX
C       Output variables: P, IP, FLAG
C
C       Parameters used internally:
C       nia   | VV - value field of a linked list describing adjacencies of
C       | vertices.
C       Size .ge. number of pairs (I,J) such that M(I,J) or
C       | M(J,I) is nonzero.
C       nia   | LV - link field of the linked list.
C       | Size = size of VV.
C       nv    | MAX - dimensioned size of VV and LV.
C
C       INTEGER IA(1), JA(1), P(1), IP(1), VV(1), LV(1), FLAG,
       * DMIN, DTHR, S, SFS, TMP, VI, VJ, VK, VL
C
C       * Initialize free storage *******************************
       VK = 1
       IF (MAX.LT.N) GO TO 109
       DO 1 S=N,MAX
       1   LV(S) = S+1
       LV(MAX) = 0
       SFS = 1
C
C       * Initialize ordering, degree, and adjacency ***********************
       DO 2 K=1,N
       VK = P(K)
       IF(VK) = K
       VV(K) = N+1
       2   LV(K) = K
       SFS = SFS + N
C* Initialize nonzero structure
C* For every vertex VK
C*** For every vertex VJ adjacent to VK
DO 8 VK=1,N
   JMIN = IA(VK)
   JMAX = IA(VK+1) - 1
   IF (JMIN.GT.JMAX) GO TO 101
   DO 7 J=JMIN,JMAX
      VJ = JA(J)
      IF (VJ.EQ.VK) GO TO 7
5 CONTINUE
8 CONTINUE

C***** Search for VJ in adjacency of VK
4 VV(VK) = VV(VK) + 1
   IF (SFS.EQ.0) GO TO 109
   LLK = SFS
   SFS = LV(SFS)
   VV(LLK) = VJ
   LV(LLK) = LV(LK)
   LV(LK) = LLK

C***** Insert VJ in adjacency of VK
C***** Search for VK in adjacency of VJ
C***** Insert VK in adjacency of VJ

C* Minimum degree algorithm with threshold search
C* Initialize vertex count and thresholds for search
I = 0
   JMIN = 1
   DTHR = 0
   DMIN = N+N
C* While uneliminated vertices exist
C*** Search for vertex VI of minimum degree
9 JMIN = MAXO (JMIN, I+1)
   DO 10 J=JMIN,N
      VI = P(J)
      IF (VV(VI).LE.DTHR) GO TO 11
10 DMIN = MINO (DMIN, VV(VI))
   JMIN = 1
   DTHR = DMIN
   DMIN = N+N
   GO TO 9
C *** Number vertex VI of minimum degree
11  **MIN = J
    I = I+1
    VJ = P(I)
    P(J) = VJ
    IP(VJ) = J
    P(I) = VI
    IP(VI) = I
    NI = 1
C *** Delete eliminated vertices from adjacency of VI
C *** For every vertex VK adjacent to VI

       LLI = VI
       KM = (VV(VI) - NI) - N
       IF (KM.LT.0) GO TO 14
       DO 13 K=1,KM
         LI = LLI
         LLI = LV(LLI)
         VK = VV(LLI)
         C ***** If VK eliminated, then delete from adjacency of VI
         IF (IP(VK).GT.I) GO TO 13
           LV(LI) = LV(LLI)
           LV(LLI) = SFS
           SFS = LLI
           LLI = LI
           GO TO 12
13  CONTINUE
C *** Eliminate vertex VI

C *** For every vertex VK adjacent to VI

       LLI = VI
       KM = (VV(VI) - NI) - N
       IF (KM.LT.0) GO TO 21
       DO 20 K=1,KM
         LI = LLI
         LLI = LV(LLI)
         VK = VV(LLI)
       14  CONTINUE
C *** Merge adjacency of VI into adjacency of VK
C *** For every vertex VJ adjacent to VI

       LLK = VK
       LJ = VI
       JM = (VV(VI) - NI) - N
       IF (JM.LT.0) GO TO 19
       DO 18 J=1,JM
         LJ = LV(LJ)
         VJ = VV(LJ)
         IF (VJ.EQ.VK) GO TO 18
15  C ***** Search for VJ in adjacency of VK
       LK = LLK
       LLK = LV(LLK)
       VI = VV(LLK)
       IF (VI.LE.VK) GO TO 17
C ***** ... while deleting eliminated vertices
       IF (IP(VL).GT.I) GO TO 16
       LV(LK) = LV(LLK)
       LV(LLK) = SFS
       SFS = LLK
       LLK = LK
16  GO TO 15
C ******** Insert VJ in adjacency of VK

17      IF (VJ.EQ.VL) GO TO 18
    VV(VK) = VV(VK) + 1
    IF (SFS.EQ.0) GO TO 109
    LLK = SFS
    SFS = LV(SFS)
    VV(LLK) = VJ
    LV(LLK) = LV(LK)
    LV(LK) = LLK
18      CONTINUE
C **** If VK of minimal degree, then number vertex VK, ...

19      IF (VV(VK).GT.VV(VI)) GO TO 20
      I = I+1
      J = IP(VK)
      VJ = P(I)
      P(J) = VJ
      IP(VJ) = J
      P(I) = VK
      IP(VK) = I
      NI = NI + 1
C ***** ... recover storage for adjacency of VK,

20      CONTINUE
C *** Update degrees of uneliminated vertices adjacent to VI
C *** For every vertex VK in adjacency of VI

21      LI = VI
      KMAX = (VV(VI) - NI) - N
      IF (KMAX.LE.0) GO TO 24
      DO 23 K=1,KMAX
      LI = LV(LI)
      VK = VV(LI)
      C ***** Update degree of VK and thresholds for cyclic search

22      DMIN = DTHR
      DTHR = VV(VK)
      JMIN = MINO (JMIN, IP(VK))
      GO TO 23
23      CONTINUE
C *** Recover storage for adjacency of VI

24      TMP = LV(VI)
      LV(VI) = SFS
      SFS = TMP
      IF (I.LT.N) GO TO 9
C
      FLAG = 0
      RETURN
C** ERROR: Null row in A
101  FLAG = N + VK
RETURN

C** ERROR: Insufficient Storage
109  FLAG = 9*N + VK
RETURN
END

-------------------------------------------------------

C*** Subroutine SRO
C*** Symmetric reordering of sparse symmetric matrix
C

SUBROUTINE SRO
  *(N, IP, IA, JA, A, TMP, Q)
C
C Input variables: N, IP, IA, JA, A
C Output variables: IA, JA, A
C
C Parameters used internally:
C nia | TMP - Initially, TMP(K) is set to the number of elements
C     | which will appear in the Kth row of M after
C     | reordering. Then TMP is initialized to IA and
C     | USED to set Q.
C nia | Size = N.
C nia | Q - Initially, Q(J) is set to the row in which A(J)
C     | (the element of the old A) will appear after
C     | reordering. Then it is set to the index of A(J) in
C     | the reordered matrix.
C     | Size = number of nonzeros in the upper triangle of M.
C
The subroutine does not rearrange the order of the rows, but
arranges each row so that the elements which will be above the
diagonal after reordering are filled in. If M(I,J) is above the
diagonal but is below the diagonal after reordering, then M(J,I)
must be filled in, so some elements will appear on different rows
after SRO is finished.

INTEGER  IP(l), IA(l), JA(l), TMP(l), Q(l), QK
REAL    A(l)
C
C ***** Initialize TMP *****************************************
  DO 1 I=1,N
      TMP(I) = 0
  C ***** For each row of A *************************************
    DO 3 I=1,N
        JMIN = IA(I)
        JMAX = IA(I+1) - 1
        IF (JMIN.GT.JMAX) GO TO 3
    C ***** For each element of the row *******************************
      DO 2 J=JMIN,JMAX
          K = JA(J)
    C ***** Adjust TMP, Q, and adjust JA if necessary ***************
        IF (IP(K).LT.IP(1)) JA(J) = I
        IF (IP(K).GE.IP(1)) K = I
        Q(J) = K
    2          TMP(K) = TMP(K) + 1
    3          CONTINUE
C ******** Set new IA and copy it into TMP
    DO 4 I=1,N
      IA(I+1) = IA(I) + TMP(I)
    4      TMP(I) = IA(I)
C ******** Q(J) gets position of A(J) after reordering
    JMIN = IA(I)
    JMAX = IA(N+1) - 1
    DO 5 J=JMIN,JMAX
      K = Q(J)
      Q(J) = TMP(K)
    5      TMP(K) = TMP(K) + 1
C ******** Reset JA and A
    DO 7 J=JMIN,JMAX
      IF (Q(J).EQ.J) GO TO 7
      K = Q(J)
      Q(J) = Q(K)
      Q(K) = K
      JA(K) = JA(J)
      JA(J) = JAK
      AK = A(J)
      A(J) = AK
    7      CONTINUE
RETURN
END
Appendix 2

Subroutines for Solving Sparse Symmetric Positive Definite Systems of Linear Equations

C*** Subroutine SDRV
C*** Driver for subroutines for solving sparse symmetric positive definite systems of linear equations

SUBROUTINE SDRV
* (N, P, IP, IA, JA, A, B, Z, NSP, ISP, RSP, PATH, FLAG)

PARAMETERS

Class abbreviations are:
 v - supplies a VALUE to the driver
 r - contains a RESULT returned by the driver
 i - is used INTERNALly by the driver
 a - is an ARRAY
 n - is an INTEGER variable
 f - is a REAL variable.

Class | Parameter
-----------------------
 v | vn N - the number of rows/columns in matrix M.
 v | vfa A - coefficient matrix for the system of linear equations Mx = b, stored in compressed form.
 v | Size = number of nonzeros in upper triangle of M (or the number of nonzeros in all of M).
 v | vna IA - pointers to the first element of each row in A.
 v | Size = N+1.
 v | vna JA - the column numbers corresponding to elements of A.
 v | Size = size of A.
 v | vna B - right-hand side for the equation Mx = b. B and Z cannot be the same vector.
 v | Size = N.

The nonzero entries of the matrix M are stored row by row in the array A. The array JA contains the corresponding column indices; i.e. if A(K) = M(I,J), then JA(K) = J. The array IA contains pointers to delimit the rows of M -- IA(I) is the index in JA and A of the first entry stored in the Ith row of M.

Only the nonzero entries on or above the diagonal need be stored. However, the subroutines will work if all nonzeros are stored.

For example, the symmetric 5 by 5 matrix

\[
\begin{bmatrix}
1 & 0 & 2 & 3 & 0 \\
0 & 4 & 0 & 0 & 0 \\
2 & 0 & 5 & 6 & 0 \\
3 & 0 & 6 & 7 & 8 \\
0 & 0 & 0 & 8 & 9
\end{bmatrix}
\]

would be stored as

\[
\begin{array}{c|c|c|c|c|c|c|c}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\hline
IA & 1 & 4 & 5 & 7 & 9 & 10 \\
JA & 1 & 3 & 4 & 2 & 3 & 4 & 4 & 5 & 5 \\
A & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
\end{array}
\]

IA(I+1) - IA(I) is the number of nonzero entries in row I, so IA(N+1), where N is the number of rows in M, is needed to determine the length of the Nth row in A.
C rna | Z  - solution vector for the equation \( Mx = b \). \( M \) and \( Z \) cannot be the same vector.
C | Size = \( N \).
C
The solution of the system is done in three stages:
C SYMFAC - The matrix \( M \) is processed symbolically to determine
C where fillin will occur during factorization.
C NUMFAC - The matrix \( M \) is factored numerically into two
C triangular matrices.
C NUMSLV - The system resulting from NUMFAC is solved.
C
For several systems with identical nonzero structures, SYMFAC
C need be done only once, then NUMFAC and NUMSLV are done for each
C system. For several systems with identical matrices \( M \) and
C different right-hand sides, SYMFAC and NUMFAC need be done only
C once, then NUMSLV is done for each right-hand side.
C
C vn | PATH - information on which subroutines are to be called.
C | Values and meanings of PATH are:
C | 1 perform SYMFAC, NUMFAC and NUMSLV.
C | 2 perform NUMFAC and NUMSLV. (SYMFAC is
C | assumed to have been done in a manner
C | compatible with the driver's storage
C | allocation.)
C | 3 perform NUMSLV only. (SYMFAC and NUMFAC
C | are assumed to have been done.)
C
C rn | FLAG - flag for error return from subroutines. Error values
C | and their meanings are:
C | 0  no error
C | \( N+I \) row \( I \) of \( A \) is null
C | \( 2N+I \) duplicate entry on row \( I \) of \( A \)
C | \( 6N+I \) storage exceeded on row \( I \) in SYMFAC
C | \( 7N+I \) storage exceeded in NUMFAC
C | \( 8N+I \) diagonal element=0 on row \( I \) in NUMFAC
C | \( 10N+1 \) ISP/RSP too small to allocate space
C | \( 11N+1 \) PATH out of bounds
C
The rows and columns of the original matrix \( M \) can be
C arbitrarily reordered before calling the driver. If no reordering
C is done, then \( P(I) = IP(I) = I \) for \( I = 1,N \). The answer vector \( Z \)
C is returned in the original order.
C
C vna | P  - the ordering of the rows (and columns) of \( M \). \( P(I) \)
C | is the number of the row of \( M \) which becomes the
C | Ith row after reordering.
C | Size = \( N \).
C
C vna | IP  - the inverse of the ordering of the rows of \( M \). That
C | is, \( IP(P(I)) = I \) for \( I = 1,N \).
C | Size = \( N \).
C
Workspace is needed to hold the factored form of the matrix
C plus various temporary vectors.
C
C na | ISP  - integer storage space divided up for various arrays
C | of the subroutines. ISP and RSP should be the
C | same array. This allows declaration of all real
C | storage to be double precision.
C
C n | NSP - dimensioned size of ISP and RSP. NSP generally
C | must be at least \( 4N+1 + 2*K \) (where \( K \) = (number of
C | nonzeros in the upper triangle of \( M \)), since ISP
and RSP must hold:

- four vectors of fixed length;
- \( JU \) (with size \( K + \text{fillin} \) - compression);
- \( U \) (with size \( K + \text{fillin} \)).

fa

RSP - real storage space divided up for various arrays of

the subroutines. ISP and RSP should be the same

array. This allows declaration of all real storage
to be double precision.

INTEGER P(1), IP(1), IA(1), JA(1), ISP(1), PATH, FLAG,

*  Q, D, U, ROW, TMP, UMAX
REAL A(1), B(1), Z(1), RSP(1)

EQUIVALENCE (ISP(1), RSP(1))

IF (PATH.LT.1 .OR. PATH.GT.3) GO TO 111

C****** Initialize and divide up temporary storage ***************

IJU = 1
IU = IJU + N
JL = IU + N+1
JU = JL + N
Q = NSF - N
JUMAX = Q - JU
IF (JUMAX.LT.0) GO TO 110

C****** Call subroutines ************

FLAG = 0
IF (PATH.GT.1) GO TO 1
CALL SSF

* (N, P, IP, IA, JA, ISP(IJU), ISP(JU), ISP(IU), JUMAX,
* RSP(Q), ISP(JL), FLAG)
IF(FLAG.NE.0) GO TO 100

C 1  D = Q - N
  U = JU + ISP(IJU+(N-1))
  ROW = Q
  UMAX = D - U
  IF (PATH.GT.2) GO TO 2
  CALL SNF

* (N, P, ISP(IJU), ISP(JU), ISP(IU), RSP(U), UMAX,
* RSP(ROW), ISP(JL), FLAG)
IF (FLAG.NE.0) GO TO 100

C 2  TMP = Q
  CALL SNS

* (N, P, RSP(D), ISP(IJU), ISP(JU), ISP(IU), RSP(U), Z, B,
* RSP(TMP))
RETURN

C ** ERROR: Error Detected in SSF, SNF, or SNS
100 RETURN
C ** ERROR: Insufficient Storage
110 FLAG = 10*N + 1
RETURN
C ** ERROR: Illegal PATH Specification
111 FLAG = 11*N + 1
RETURN

END

C

-----------------------------------------------
I. SUBROUTINE NAMES

Subroutine names are of the form Sxx where:

1) the first letter is S for symmetric matrices;
2) the second letter is either S for symbolic or N for numerical processing;
3) the third letter is either F for factorization or S for solution.

II. CALLING SEQUENCES

The input matrix can be processed with an ordering subroutine before using the remaining subroutines. If this is done and only the upper triangle of M is being stored, SRO should be called to reorder the matrix into symmetric form before using the other subroutines. If an ordering subroutine is not used, set P(I) = IP(I) = I for I=1,N. Then the calling sequence is

SSF (symbolic factorization)
SNF (numerical factorization)
SNS (called once for each right-hand side).

III. STORAGE OF SPARSE MATRICES

The nonzero entries of the matrix M are stored row by row in the array A. The array JA contains the corresponding column indices; i.e. if A(K) = M(I,J), then JA(K) = J. The array IA contains pointers to delimit the rows of M -- IA(I) is the index in JA and A of the first entry stored in the Ith row of M.

Only the nonzero entries on or above the diagonal need be stored. However, the subroutines will work if all nonzeros are stored.

For example, the symmetric 5 by 5 matrix

| 1 0 2 3 0 |
| 0 4 0 0 0 |
| 2 0 5 6 0 |
| 0 3 0 6 7 8 |
| 0 0 0 8 9 |

would be stored as

| IA | 1 2 3 4 5 6 7 8 9 |
|-----|
| IA(I+1) - IA(I) | is the number of nonzero entries in row I, so IA(N+1), where N is the number of rows in M, is needed to determine the length of the Nth row in A.
| IA(N+1) | is the number of rows in M.

The unit triangular matrix U is stored in a similar fashion using the arrays IU, JU, and U except that an additional vector IJU is used to compress storage of JU. IJU(K) points to the starting location in JU of entries for the Kth row. Compression occurs in two ways. First, if a row I was merged into the current row K, and the number of elements merged in from row I (some tail portion of row I) is the same as the final length of row K, then the Kth row and the tail are identical and IJU(K) can point to the start of the tail. Second, if some tail portion of the K-1st row equals the head of the Kth row, then IJU(K) can point to the start of that tail section. For example, the nonzero structure of
might be stored, ignoring the diagonal, as
\[
\begin{vmatrix}
1 & 2 & 3 & 4 & 5 & 6 \\
1 & 4 & 6 & 7 & 8 & \ \\
3 & 4 & 5 & 4 & \\
1 & 2 & 4 & 3 & .
\end{vmatrix}
\]

The diagonal entries of \( U \) are assumed to be equal to one and are not stored. The array \( D \) contains reciprocals of entries of the diagonal matrix in the \( U\) DU decomposition.

IV. ADDITIONAL STORAGE SAVINGS

In SSF and SNF, \( P \) and \( IP \) can be the same vector in the calling sequences if no reordering of the matrix has been done (i.e. \( P(I) = IP(I) = I \) for \( I=1,N \)).

In SNS, \( B \) and \( Z \) can be the same; however, the right-hand side \( B \) will be destroyed.

V. PARAMETERS

Following is a list of parameters to the programs. Names are uniform among the various subroutines. Class abbreviations are:

- \( v \) - supplies a VALUE to the subroutine
- \( r \) - contains a RESULT returned by the subroutine
- \( i \) - is used INTERNALLY by the subroutine
- \( a \) - is an ARRAY
- \( n \) - is an INTEGER variable
- \( f \) - is a REAL variable.

<table>
<thead>
<tr>
<th>Class</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( fva )</td>
<td>A</td>
<td>coefficient matrix for the system of linear equations ( Mx = b ), stored in compressed form. Size = either the number of nonzeros in the upper triangle of ( M ), or the number of nonzeros in all of ( M ) (see section III).</td>
</tr>
<tr>
<td>( fva )</td>
<td>B</td>
<td>right-hand side for the equation ( Mx = b ). Size = ( N ).</td>
</tr>
<tr>
<td>( fvara )</td>
<td>D</td>
<td>inverse of diagonal matrix in ( U) DU factorization (also used for temporary results in SNF). Size = ( N ).</td>
</tr>
<tr>
<td>( nvra )</td>
<td>IA</td>
<td>pointers to first elements of each row in ( A ). Size = ( N+1 ).</td>
</tr>
<tr>
<td>( nr )</td>
<td>FLAG</td>
<td>flag for error return from subroutines. Error values and their meanings are: 0 - no error N+1 - row I of ( A ) is null 2N+1 - duplicate entry on row I of ( A ) 6N+1 - JU storage exceeded on row I 7N+1 - U storage exceeded 8N+1 - zero diagonal element on row I</td>
</tr>
<tr>
<td>( nvra )</td>
<td>IJU</td>
<td>pointers to the first elements of each row in ( JU ), used to compress storage of ( JU ). Size = ( N ).</td>
</tr>
<tr>
<td>( nva )</td>
<td>IP</td>
<td>inverse of the ordering of the rows of ( M ). For example, if row 1 is the 5th row after reordering, then ( IP(1) = 5 ). Size = ( N ).</td>
</tr>
</tbody>
</table>
C nvra IU - pointers to the first elements of each row in U.
C Size = N+1.
C nvra JA - column numbers corresponding to elements of A.
C Size = size of A.
C nvra JU - column numbers corresponding to elements of U.
C Size = size of U - compression.
C nv JUMAX - declared dimension of JU.
C nv N - number of rows/columns in matrix M.
C nv JA - column numbers corresponding to elements of A.
C Size = size of A.
C nv JU - column numbers corresponding to elements of U.
C Size = size of U - compression.
C nv JUMAX - declared dimension of JU.
C nv N - number of rows/columns in matrix M.
C nvra P - ordering of rows (and columns) of M. P(I) is
C the number of the row of M which becomes the Ith
C row after reordering.
C Size = N.
C nvra U - upper triangular matrix resulting from the
C factorization of M, stored in compressed form.
C Size = number of nonzeros in upper triangle of M
C plus fillin (IU(N+I)-1 after SSF).
C nv UMAX - declared dimension of U.
C fra Z - solution vector for the equation Mx = b.
C Size = N.

C*** Subroutine SSF

C*** Symbolic Ut-D-U factorization of sparse symmetric matrix

SUBROUTINE SSF
  *(N, P, IP, IA, JA, IJU, JU, IU, JUMAX, Q, JL, FLAG)

C Input variables: N, P, IP, IA, JA, JUMAX
C Output variables: IJU, JU, IU, FLAG

C Parameters used internally:
C
C nia JL - linked list of rows to be merged. If the Kth row is
C being processed, JL(K) contains the number of the
C first row to be merged with the Kth row, JL(JL(K))
C is the number of the second row, etc.
C Size = N.
C nia Q - Suppose M' is the result of reordering M. If
C processing of the Kth row of M' (hence the Kth row
C of U) is being done, Q(J) is initially nonzero if
C M'(K,J) is nonzero and above the diagonal. Since
C values need not be stored, each entry points to the
C next nonzero and Q(K) points to the first. N+1
C indicates the last element. For example, if N=9 and
C the 5th row of M' is
C 0 x 0 x 0 0 0 x 0
C then Q will initially be
C a a a a 8 a a 10 a
C (a - arbitrary).
C As the algorithm proceeds, other elements of Q are
C inserted in the list because of fillin.
C Size = N.

C Internal variables:
C JUMIN, JUPT - are the indices in JU of the first and last
C elements in either the last or the current row.
C LMAX - length of longest row merged into Q.
C LUI - number of elements in a row to be merged into Q.
C LUK - number of elements in the current row (Q).
C

INTEGER P(l), IP(l), IA(l), JA(l), IJU(l), JU(l), IU(l),
* Q(l), JL(l), FLAG, VJ, QM

C

C****** Initialize ************************************************

JMIN = 1
JUPTR = 0
IU(1) = 1
DO 1 K=1,N
1 JL(K) = 0

C

C****** For each row ************************************************

DO 15 K=1,N

C****** Initialize Q to structure of Kth row above diagonal *******

LUK = 0
Q(K) = N+1
JMIN = IA(P(K))
JMAX = IA(P(K)+1) - 1
IF (JMIN.GT.JMAX) GO TO 101
DO 3 J=JMIN,JMAX
VJ = IP(JA(J))
IF (VJ.LE.K) GO TO 3
QM = K
2 M = QM
QM = Q(M)
IF (QM.LT.VJ) GO TO 2
IF (QM.EQ.VJ) GO TO 102
LUK = LUK+1
Q(M) = VJ
Q(VJ) = QM
3 CONTINUE

C

C****** Compute fillin for Q by ************************************************

IMAX = 0
IJU(K) = JUPTR
I = K

C****** Linking through JL and ************************************************

4 I = JL(I)
IF (I.EQ.0) GO TO 8
LUI = IU(I+1) - (IU(I)+1)
JMIN = IJU(I) + 1
JMAX = IJU(I) + LUI
IF (LUI.LE.IMAX) GO TO 5
IMAX = LUI
IJU(K) = JMIN
5 QM = K

C****** Merging each row with Q ************************************************

DO 7 J=JMIN,IMAX
VJ = JU(J)
6 M = QM
QM = Q(M)
IF (QM.LT.VJ) GO TO 6
IF (QM.EQ.VJ) GO TO 7
LUK = LUK+1
Q(M) = VJ
Q(VJ) = QM
QM = VJ
7 CONTINUE

GO TO 4
C ****** Check if row duplicates another. If not ********************
8 IF (LUK.EQ.LMAX) GO TO 14
C ****** see if tail of K-1st row matches head of Kth **************
   IF (JUMIN.GT.JUPTR) GO TO 12
      I = Q(K)
      DO 9 JMIN=JMIN,JUPTR
           IF (JU(JMIN)-I) 9, 10, 12
5 CONTINUE
   GO TO 12
10 IJU(K) = JMIN
   DO 11 J=JMIN,JUPTR
      IF (JU(J).NE.I) GO TO 12
      I = Q(I)
   CONTINUE
   JUPTR = JMIN - 1
C ****** Set Kth row of U to Q **************************************
12 JMIN = JUPTR + 1
   JUPTR = JUPTR + LUK
   IF (JUPTR.GT.JUMAX) GO TO 106
      I = K
   DO 13 J=JMIN,JUMAX
      I = Q(I)
13 JU(J) = I
   IJU(K) = JUMIN
C ****** If more than one element in row, adjust JL *****************
14 IF (LUK.LE.1) GO TO 15
      I = JU(IJU(K))
      JL(K) = JL(I)
      JL(I) = K
15 IU(K+1) = IU(K) + LUK
C  
   FLAG = 0
   RETURN
C C ** ERROR: Null Row in A  
101 FLAG = N + P(K)
   RETURN
C C ** ERROR: Duplicate Entry in A  
102 FLAG = 2*N + P(K)
   RETURN
C C ** ERROR: Insufficient Storage for JU  
106 FLAG = 6*N + K
   RETURN
END
C

C

C*** Subroutine SNF
C*** Numerical U-D-U factorization of sparse symmetric positive
C definite matrix
C
SUBROUTINE SNF
*
(N, P, IP, IA, JA, A, IJU, JU, U, UMAX, IL, JL, FLAG)

C Input variables:  N, P, IP, IA, JA, A, IJU, JU, IU
C Output variables:  D, U, FLAG
C
Parameters used internally:
C
niva D - If the Kth row of U is being computed, D(l) through
| D(K-1) contain reciprocals of the entries of the
| diagonal matrix D from the decomposition. The
| remainder of D is initialized to the structure of
| the Kth row of M (after reordering) and is adjusted
| to become the Kth row of U.
C
niva IL - IL(l) points to the first element of the Ith row to be
| used in adjusting the current row.
| Size = N.
C niva JL - linked list of rows to be used in adjusting the current
| row.  If the Kth row is being processed, JL(K)
| contains the number of the first row to be used with
| the Kth row, JL(JL(K)) is the number of the second
| row, etc.
| Size = N.

INTEGER P(l), IP(l), IA(l), JA(l), IJU(l), JU(l), IU(l),
* UMAX, IL(l), JL(l), FLAG, VK, VJ
DIMENSION A(l), D(l), U(l)
C
****** Initialize JL, check storage ****************************
IF (IU(N+1)-l .GT. UMAX) GO TO 107
DO 1 K=l,N
  1  JL(K) = 0
C
****** For each row  ********************************************
DO 10 K=l,N
C
****** Initialize D on and above the diagonal  ******************
  JMIN = IU(K)
  JMAX = IU(K+l) - l
  IF (JMIN.GT.JMAX) GO TO 3
  MU = IJU(K) - IU(K)
  DO 2 J=JMIN,JMAX
    2  D(JU(MU+J))) = 0
  3  D(K) = 0
  VK = P(K)
  JMIN = IA(VK)
  JMAX = IA(VK+l) - l
  DO 4 J=JMIN,JMAX
    4  VJ = IP(JA(J))
    IF (K.LE.VJ) D(VJ) = A(J)
  CONTINUE
C

C For each element in lower triangle to be eliminated

  *  \( D_K = D(K) \)
  *  \( \text{NXTI} = \text{JL}(K) \)
  *  \( I = \text{NXTI} \)
  *  IF (I.EQ.0) GO TO 8

C Change D and adjust IL and JL

  *  \( \text{NXTI} = \text{JL}(I) \)
  *  \( \text{UKIDI} = -U(\text{IL}(I)) \times D(I) \)
  *  \( D_K = D_K + \text{UKIDI} \times U(\text{IL}(I)) \)
  *  \( U(\text{IL}(I)) = \text{UKIDI} \)
  *  \( \text{JMIN} = \text{IL}(I) + 1 \)
  *  \( \text{JMAX} = I(U(I+1)) - 1 \)
  *  IF (\text{JMIN}.GT.\text{JMAX}) GO TO 7
  *  \( \text{MU} = I(U(I)) - I(U(I)) \)
  *  DO 6 J=\text{JMIN},\text{JMAX}

\[
D(JU(MU+J)) = D(JU(MU+J)) + \text{UKIDI} \times U(J)
\]

  *  \( \text{IL}(I) = \text{JMIN} \)
  *  \( J = JU(MU+JMIN) \)
  *  \( \text{JL}(I) = \text{JL}(J) \)
  *  \( \text{JL}(J) = 1 \)

  *  7 GO TO 5

C

C For each element in lower triangle to be eliminated

  *  \( D(K) = D(K) \)
  *  \( \text{IL}(K) = JMIN \)
  *  \( \text{JL}(K) = \text{JL}(I) \)
  *  \( \text{JL}(I) = K \)

  *  10 CONTINUE

C

\[ \text{FLAG} = 0 \]

RETURN

C ** ERROR: Insufficient Storage for U

  *  \( \text{FLAG} = 7*\text{N} + 1 \)

RETURN

C ** ERROR: Zero Pivot

  *  \( \text{FLAG} = 8*\text{N} + K \)

RETURN

END
C
C
C*** Subroutine SNS
C*** Numerical solution of sparse symmetric positive definite system of
C linear equations given Ut-D-U factorization
C
SUBROUTINE SNS
* (N, P, D, IJU, JU, U, Z, B, TMP)

C Input variables: N, P, D, IJU, JU, U, B
C Output variables: Z
C
Parameters used internally:
C fia | TMP - vector which gets result of solving Ut Dy = b.
C | Size = N.
C
INTEGER P(I), IJU(1), JU(1), IU(1)
REAL D(1), U(1), Z(1), B(1), TMP(1)
C
C ***** Initialize TMP to the reordered B ****************************
DO 1 K=1,N
1 TMP(K) = B(P(K))
C ***** Solve Ut Dy = b by forward substitution ********************
DO 3 K=1,N
   TMPK = TMP(K)
   JMIN = IU(K)
   JMAX = IU(K+1) - 1
   IF (JMIN.GT.JMAX) GO TO 3
   MU = IJU(K) - JMIN
   DO 2 J=JMIN,JMAX
      TMP(JU(MU+J)) = TMP(JU(MU+J)) + U(J) * TMPK
   2 SUM = SUM + U(J) * TMP(JU(MU+J))
   TMP(K) = TMPK * D(K)
C
C ***** Solve Ux = y by back substitution ****************************
K = N
DO 6 I=1,N
   SUM = TMP(K)
   JMIN = IU(K)
   JMAX = IU(K+1) - 1
   IF (JMIN.GT.JMAX) GO TO 5
   MU = IJU(K) - JMIN
   DO 4 J=JMIN,JMAX
      SUM = SUM + U(J) * TMP(JU(MU+J))
   4 TMP(K) = SUM
   Z(P(K)) = SUM
   K = K-1
6 RETURN
END
**Appendix 3**

**Test Driver for Sparse Symmetric Matrix Package**

C*** Program STST
C*** Test Driver for Symmetric Codes in Yale Sparse Matrix Package

Variables:

NG - size of grid used to generate test problem.

N  - number of variables and equations (= NG x NG).

IA - INTEGER one-dimensional array used to store row pointers to JA and A; DIMENSION = N+1.

JA - INTEGER one-dimensional array used to store column indices of nonzero elements of (upper triangle of) M;
     DIMENSION = number of nonzero entries in (upper triangle of) M.

A - REAL one-dimensional array used to store nonzero elements of (upper triangle of) M; DIMENSION = number of nonzero entries in (upper triangle of) M.

X - REAL one-dimensional array used to store solution x; DIMENSION = N.

B - REAL one-dimensional array used to store right-hand-side b
    DIMENSION = N.

P - INTEGER one-dimensional array used to store permutation of rows and columns for reordering linear system;
    DIMENSION = N.

IP - INTEGER one-dimensional array used to store inverse of permutation stored in P; DIMENSION = N.

NSP - declared dimension of one-dimensional arrays ISP and RSP.

ISP - INTEGER one-dimensional array used as working storage (equivalenced to RSP); DIMENSION = NSP.

RSP - REAL one-dimensional array used as working storage (equivalenced to ISP); DIMENSION = NSP.

INTEGER IA(101), JA(500), P(100), IP(100), ISP(1500),
CASE, PATH, FLAG, APTR, VP, VQ, X, XMIN, XMAX, Y, YMIN, YMAX
REAL A(500), Z(100), B(100), RSP(1500)
EQUIVALENCE (ISP(1), RSP(1))
DATA NSP/1500/, EPS/1E-5/

INDEX(I,J) = NG*1 + J - NG

NG = 3
N = NG*NG
C***** For CASE=1 we store the entire matrix, for CASE=2 we store
only the upper triangular part
DO 5 CASE=1,2
C
C***** Set up matrix for five point finite difference operator
******
APTR = 1
DO 2 I=1,NG
  DO 2 J=1,NG
    VP = INDEX (I, J)
    P(VP) = VP
    IP(VP) = VP
    IA(VP) = APTR
    SUM = 0
    XMIN = MAXO ( 1, I-1)
    XMAX = MINO (NG, I+1)
    YMIN = MAXO ( 1, J-1)
    YMAX = MINO (NG, J+1)
    DO 1 X=XMIN,XMAX
      DO 1 Y=YMIN,YMAX
        IF ((X-I) * (Y-J) .NE. 0) GO TO 1
        VQ = INDEX(X, Y)
        JA(APTR) = VQ
        A(APTR) = 4
        IF (VP .NE. VQ) A(APTR) = -1
        SUM = SUM + A(APTR) * VQ
    1 CONTINUE
  B(VP) = SUM
2 CONTINUE
IA(N+1) = APTR
NZA = IA(N+1) - 1
C
C***** Output original array A
******
IF (CASE.EQ.1) PRINT 1001, NG,NG
1001 FORMAT ('FIVE-POINT OPERATOR ON ', I1, ' BY ', I1, ' GRID'
* ' (ALL ENTRIES OF MATRIX STORED) ')
IF (CASE.EQ.2) PRINT 1002, NG,NG
1002 FORMAT ('FIVE-POINT OPERATOR ON ', I1, ' BY ', I1, ' GRID'
* ' (ONLY ENTRIES OF UPPER TRIANGLE STORED) ')
PRINT 1003, (IA(I),I=1,N), IA(N+1)
1003 FORMAT ('COEFFICIENT MATRIX: '
* ' IA (INDICES OF FIRST ELEMENTS IN ROWS)'
* ' (1015))
PRINT 1004, (I,JA(I),A(I), I=1,NZA)
1004 FORMAT ('JA A '
* ' I COLUMN INDICES MATRIX'
* ' (13,110,F16.5))
PRINT 1005, (B(I), I=1,N)
1005 FORMAT ('RIGHT HAND SIDE B: '
* ' (5F10.5))
C
C ***** Call ODRV
******
FLAG = 0
PATH = CASE
CALL ODRV
* (N, IA,JA,A, P,IP, NSP, RSP, PATH, FLAG)
IF (FLAG.NE.0) GO TO 101
C
C***** Output reordered array A
******
PRINT 1006, (I,P(I),IP(I), I=1,N)
1006 FORMAT ('/ ROW/COLUMN ORDERING FROM ODIRV: /', * P * / I ROW/COLUMN ORDERING INVERSE ORDERING * / (I3, I10, 120))
1007 IF (CASE.EQ.2) PRINT 1007, (IA(I), I=1,N), IA(N+1)
1008 FORMAT ('/ REORDERED COEFFICIENT MATRIX: /', * / IA (INDICES OF FIRST ELEMENTS IN ROWS) /', * / (1015))
1009 IF (CASE.EQ.2) PRINT 1008, (I,JA(I),A(I), I=1,NZA)
1010 FORMAT ('/ JA A ' /', * / I COLUMN INDICES MATRIX /', * / (13, I10, F16.5))
C
C ****** Call SDRV ***********************************************
CALL SDRV
* (N, P, IP, JA, A, B, Z, NSP, ISP, RSP, PATH, FLAG)
IF (FLAG.NE.0) GO TO 102
C
C ****** Calculate error *********************************************
SUM = 0
DO 4 I=1,N
  4 SUM = SUM + ((Z(I)-I)/I)**2
RMS = SQRT(SUM/N)
C
C ****** Output solution and error measure *****************************
PRINT 1009, (Z(I),I=1,N)
1011 IF (RMS.LE.EPS) PRINT 1010, RMS
1012 FORMAT ('/ SOLUTION CORRECT: RMS ERROR = ', 1PE8.2)
1013 IF (RMS.GT.EPS) PRINT 1011, RMS
1014 FORMAT ('/ SOLUTION INCORRECT: RMS ERROR = ', 1PE8.2)
C
5 CONTINUE
STOP
C
C ****** Error messages ***********************************************
101 PRINT 1012, FLAG
1012 FORMAT ('/ ERROR IN ODIRV: FLAG = ', I5)
STOP
C
102 PRINT 1013, FLAG
1013 FORMAT ('/ ERROR IN SDRV: FLAG = ', I5)
STOP
END
Appendix 4
Sample Output From Test Driver

*** FIVE-POINT OPERATOR ON 3 BY 3 GRID
(ALL ENTRIES OF MATRIX STORED)

COEFFICIENT MATRIX:

IA (INDICES OF FIRST ELEMENTS IN ROWS)
1  4  8 11 15 20 24 27 31 34

<table>
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<th>COLUMN INDICES</th>
<th>MATRIX</th>
</tr>
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RIGHT HAND SIDE B:
-2.00000 -1.00000 4.00000 3.00000 0.00000
7.00000 16.00000 11.00000 22.00000
ROW/COLUMN ORDERING FROM ODRV:

<table>
<thead>
<tr>
<th>P</th>
<th>ROW/COL ORDERING</th>
<th>IP</th>
<th>INVERSE ORDERING</th>
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</table>

SOLUTION FROM SDRV:

1.00000 2.00000 3.00000 4.00000 5.00000
6.00000 7.00000 8.00000 9.00000

SOLUTION CORRECT: RMS ERROR = 1.39E-08

*** FIVE-POINT OPERATOR ON 3 BY 3 GRID
(ONLY ENTRIES OF UPPER TRIANGLE STORED)

COEFFICIENT MATRIX:

IA (INDICES OF FIRST ELEMENTS IN ROWS)
1 4 7 9 12 15 17 19 21 22

<table>
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<tr>
<th>IA</th>
<th>COLUMN INDICES</th>
<th>MATRIX</th>
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</table>

RIGHT HAND SIDE B:

-2.00000 -1.00000 4.00000 3.00000 0.00000
7.00000 16.00000 11.00000 22.00000
ROW/COLUMN ORDERING FROM ODRV:

<table>
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<tr>
<th>P</th>
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<td>8</td>
</tr>
</tbody>
</table>

REORDERED COEFFICIENT MATRIX:

IA (INDICES OF FIRST ELEMENTS IN ROWS)
1 4 5 8 9 13 15 18 19 22

JA (COLUMN INDICES)

<table>
<thead>
<tr>
<th>I</th>
<th>COLUMN INDICES MATRIX</th>
</tr>
</thead>
<tbody>
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</table>

SOLUTION FROM SDRV:
1.00000 2.00000 3.00000 4.00000 5.00000
6.00000 7.00000 8.00000 9.00000

SOLUTION CORRECT: RMS ERROR = 1.39E-08