ALGORITHM 572
Solution of the Helmholtz Equation for the Dirichlet Problem on General Bounded Three-Dimensional Regions [D3]

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DESCRIPTION

This algorithm provides an approximate solution to the Helmholtz equation

$$-\Delta u + cu = g \qquad \text{in } \Omega$$

with a Dirichlet boundary condition

$$u = f \qquad \text{on } \Gamma, \text{ the boundary of } \Omega.$$

Here Ω, a three-dimensional bounded region, c, an arbitrary real constant (positive, negative, or zero), and the functions f and g are specified by the user. The Laplace operator Δ is in Cartesian coordinates.

A second-order accurate finite-difference method is used to discretize the Helmholtz equation. The resulting linear system of equations is reduced to a capacitance matrix equation that is solved approximately by a conjugate gradient

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method. We sketch the basic ideas below, but a detailed discussion of this and similar methods can be found in [1].

To perform the discretization, the region Ω is embedded in a cube and a uniform rectangular finite-difference grid is imposed. A simple seven-point difference approximation is used for all mesh points except those that are in Ω and are near the boundary Γ. For these boundary neighbors, second-order accurate equations incorporating the boundary data are used. The resulting difference scheme is known as the Shortley-Weller method. Thus the discrete system of equations has a matrix that differs from that for a Helmholtz problem on the cube only in those rows that correspond to points near Γ. We take advantage of this by reformulating the problem as one of dimension equal to the number of boundary neighbors rather than the number of mesh points in the region. The resulting linear system is the capacitance matrix equation. In our implementation this reduced equation is then solved using an iterative algorithm, the conjugate gradient method. A special scaling method, based on so-called discrete dipoles, is used to enhance the convergence. A fast Poisson solver on the cube is one of the components necessary to evaluate the product of the capacitance matrix with a given vector.

Let NX, NY, and NZ be the numbers of mesh points in the cube along the three coordinate axes, where NX and NY are powers of 2. We denote the number of mesh points in Ω with at least one of their six nearest neighbors on or outside the boundary Γ by IPP1 + IPP2, where IPP2 points have two such neighbors along at least one coordinate mesh line. The program requires as input certain scalar parameters, the coordinates of each of the IPP1 + IPP2 points and their distances to the boundary along mesh lines, the values of the Dirichlet data f at points of intersection of mesh lines and the boundary Γ, and the value of the function g at mesh points in Ω. The user communicates with the package through the subroutine HELM3D. A complete description of the input parameters is given in the comments at the beginning of this subroutine.

HELM3D controls the conjugate gradient iteration and calls upon a fast solver (CUBE) and subroutines UTAMLT, UTATRN, BNDRY, VMULT, and VTRANS to perform the necessary matrix-vector products. CUBE solves the Helmholtz equation on a cube using fast discrete Fourier transform routines RFORT and FORT to reduce the systems to tridiagonal form. The resulting linear systems are solved by a Toeplitz method, and then an inverse Fourier transform is performed. RFORT and FORT were provided by Dr. W. Proskurowski, who has modified a code written by Dr. J. Cooley. HELM3D also employs an error-checking module HELMCK to check the input data. It diagnoses errors in the integer parameters, missing boundary points, and inconsistencies in the given boundary data.

The program requires two arrays of dimension NX $\times$ NY $\times$ NZ (one if $g = 0$), four integer and six real arrays of dimension IPP1 + 2 * IPP2, and one real array of dimension max(IPP1 + 2 * IPP2, NX * NZ, NY * NZ). Each conjugate gradient iteration requires time proportional to NX * NY * NZ * LOG (NX * NY), and the number of iterations will usually be small unless a value of c is used that makes the discrete Helmholtz operator almost singular. Double precision is required on machines with a short word length.

Data on timing for many sample problems are given in [1]. As an example, a discrete Laplace problem on a cube with a sphere cut out of it having 10464 mesh points and embedded in a cube of dimension 32 × 32 × 24 required 84K words of storage and 171 seconds on a CDC 6600 (FTN compiler, OPT = 2) to find a solution of the linear system with a maximum error equal to 0.55×10^{-3} of the maximum value of the solution.

A sample driver is included with the algorithm. Possible enhancements to the algorithm are discussed in [1].

REFERENCES

1. O'LEARY, D. P., AND WIDLUND, O. Capacitance matrix methods for the Helmholtz equation on general three dimensional regions. Courant Inst. Rep. COO-3077-155, New York, Oct. 1978; also *Math. Comp. 33* (1979), 849–879.

ALGORITHM

[A part of the listing is printed here. The complete listing is available from the ACM Algorithms Distribution Service (see page 257 for order form).]

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      SUBROUTINE HELM3D (MODE, W, GG, NXDIM, NYDIM, NZDIM, IPP1, IPP2, DELTA, NNX
     1, NNY, NNZ, NIPDIM, NAPDIM, ICOORD, INDORD, CC, NIT, EPS, S, R, P, AP, IER)
      INTEGER MODE, NXDIM, NYDIM, NZDIM, IPP1, IPP2, NNX, NNY, NNZ, NIPDIM, ICOORD
     1(3, NIPDIM), INDORD(NIPDIM), NIT, IER
      REAL W(NXDIM, NYDIM, NZDIM), GG(NXDIM, NYDIM, NZDIM), DELTA(3, NIPDIM), CC
     1, EPS, S(NIPDIM), R(NIPDIM), P(NIPDIM), AP(NAPDIM)
C
C        THIS PROGRAM WAS DEVELOPED BY DIANNE P O'LEARY AND OLOF WIDLUND
C        THIS IS  VERSION MD2,   OCTOBER,  1979
C
C        THIS PROGRAM SOLVES THE DIRICHLET PROBLEM FOR THE
C        HELMHOLTZ EQUATION OVER A GENERAL BOUNDED 3 DIMENSIONAL
C        REGION IMBEDDED IN A UNIT CUBE
C
C         -W    - W    - W    + CC*W = G1    IN THE REGION
C           XX     YY     ZZ
C
C          W = F                            ON THE BOUNDARY
C
C        WHERE F AND G1 ARE GIVEN FUNCTIONS OF X, Y, AND Z, AND  CC   IS
C        A REAL CONSTANT   THE BOUNDARY IS ARBITRARY   THE PROGRAM
C        PROVIDES A SOLUTION OF THE WELL KNOWN SHORTLEY-WELLER
C        APPROXIMATION OF THE DIFFERENTIAL EQUATION   THE MESH IS UNIFORM
C        IN EACH COORDINATE DIRECTION AND A SIMPLE SEVEN POINT FORMULA
C        IS USED FOR INTERIOR MESH POINTS   A CAPACITANCE MATRIX
C        METHOD,  WITH DISCRETE DIPOLES,  IS USED   THE CAPACITANCE
C        MATRIX EQUATION IS FORMULATED AS A LEAST SQUARES PROBLEM
C        AND SOLVED USING THE CONJUGATE GRADIENT METHOD.
C
C      REFERENCES
C
C        O'LEARY AND WIDLUND, CAPACITANCE MATRIX METHODS
C        FOR THE HELMHOLTZ EQUATION ON GENERAL 3-DIMENSIONAL
C        REGIONS,  NYU-DOE REPORT  COO-3077-155, OCTOBER, 1978,
C        MATH  COMP  33, 1979 849-880
C
C        PROSKUROWSKI AND WIDLUND,  MATH COMP  30, 1976 443-468.
C        ALSO  NYU-DOE REPORT
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C
C       PROSKUROWSKI, LAWRENCE BERKELEY LAB REPORTS AND
C       "NUMERICAL SOLUTION OF HELMHOLTZ'S EQUATION BY
C       IMPLICIT CAPACITANCE MATRIX METHODS," ACM TRANS
C       ON MATH  SOFTWARE 5, 1979 36-49.
C
C       SHIEH, MRC-WISCONSIN REPORTS AND NUMER. MATH  29
C       1978 307-327
C
C
C     MACHINE DEPENDENT FEATURES
C
C       THIS PROGRAM SHOULD BE CONVERTED TO DOUBLE PRECISION
C       IF IT IS TO BE USED ON COMPUTERS WITH SHORT WORD
C       LENGTH ,SUCH AS IBM 360/370
C
C
C     GENERAL DESCRIPTION OF THE PARAMETERS.
C
C       INTEGER VALUES
C         DIMENSIONS OF ARRAYS  (NXDIM, NYDIM, NZDIM,
C             NIPDIM, NAPDIM)
C         NUMBER OF MESH POINTS IN CUBE  (NNX X NNY X
C             NNZ)
C         NUMBER OF POINTS IN REGION ADJACENT TO BOUNDARY
C             (IPP1, IPP2)
C         MAXIMUM NUMBER OF ITERATIONS ALLOWED  (NIT)
C         ERROR CODE  (IER)
C         CODE TO CONTROL PROGRAM OPTIONS  (MODE)
C
C       REAL VALUES
C         HELMHOLTZ CONSTANT  (CC)
C         CONVERGENCE TOLERANCE  (EPS)
C
C       INTEGER ARRAYS
C         COORDINATES OF POINTS IN REGION ADJACENT TO
C              BOUNDARY ('IRREGULAR POINTS')  (ICOORD)
C         WORK SPACE  (INDORD)
C
C       REAL ARRAYS
C         G1  VALUES  (GG)
C         BOUNDARY VALUES  (R, P, AP)
C         DISTANCES FROM IRREGULAR POINTS TO BOUNDARY
C             (DELTA)
C         WORK SPACE  (W, S)
C
C
C       TOTAL ARRAY SPACE NEEDED
C         REAL    2  NXDIM * NYDIM * NZDIM  (1  IF  G1=0)
C                 6  NIPDIM
C                 1  NAPDIM
C         INTEGER
C                 4  NIPDIM
C
C         WHERE  NXDIM  GE  NNX,   NYDIM . GE  NNY,
C                NZDIM  GE  NNZ,
C                NIPDIM  GE  IPP1 + 2 * IPP2,
C                NAPDIM  GE  MAX (IPP1+2*IPP2, NNX*NNZ,
C                                 NNY*NNZ)
C
C
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C      NOTE
C
C        IN THIS DOCUMENTATION,  NN  REFERS TO  NNX,  NNY,  OR  NNZ
C        AS APPROPRIATE, AND SIMILARLY  H REFERS TO  HX,  HY,  OR  HZ.
C        THE MESH POINT (X,Y,Z) IS SAID TO HAVE 6 NEIGHBORS.
C           (X+HX,Y,Z),  (X-HX,Y,Z),  (X,Y+HY,Z),  (X,Y-HY,Z),
C           (X,Y,Z+HZ),  AND (X,Y,Z-HZ)
C        A MESH POINT IS CALLED IRREGULAR IF IT IS IN THE INTERIOR OF
C        THE REGION AND AT LEAST ONE OF ITS SIX NEIGHBORS IS ON OR
C        OUTSIDE THE BOUNDARY

C    ON INPUT
C     -- MODE =  1 IF THE REGION HAS BEEN CHANGED FROM THE PREVIOUS CALL
C                  AND  G1=0
C                2 IF THE REGION HAS BEEN CHANGED FROM THE PREVIOUS CALL
C                  AND  G1  IS NONZERO
C                3 IF THE REGION IS THE SAME AS ON THE PREVIOUS CALL
C                  AND  G1=0
C                4 IF THE REGION IS THE SAME AS ON THE PREVIOUS CALL
C                  AND  G1  IS NONZERO
C                5 IF THE PROBLEM IS THE SAME AS ON THE  PREVIOUS CALL,
C                  G1=0,  AND THE ONLY CHANGE IS THAT  EPS  AND/OR  NIT
C                  MAY HAVE BEEN CHANGED
C                6 IF THE PROBLEM IS THE SAME AS ON THE PREVIOUS CALL,
C                  G1  IS NONZERO, AND THE ONLY CHANGE IS THAT  EPS
C                  AND/OR  NIT  MAY HAVE BEEN CHANGED
C         IF  MODE = 3,4,5, OR 6  DELTA,  ICOORD,  INDORD,  NXDIM,
C         NYDIM,  NZDIM,  NNX,  NNY,  NNZ,  IPP1,  AND IPP2  MUST BE
C         UNCHANGED FROM THE PREVIOUS CALL  THE CURRENT VALUE OF  S
C         WILL BE USED AS THE INITIAL GUESS FOR THE DIPOLE STRENGTHS
C         (S=0 WILL BE USED IF MODE=1 OR 2 )
C         TO IMPROVE THE ACCURACY OF A PREVIOUSLY CALCULATED SOLUTION,
C         USE  MODE=5  OR MODE=6  IF ROUNDOFF IS NOT SUSPECTED.  IF
C         ROUNDOFF IS SUSPECTED, REINITIALIZE THE BOUNDARY VALUES IN  R,
C         AP,  AND  P,  AND USE  MODE = 3 TO FORCE THE RESIDUAL TO BE
C         RECOMPUTED, IF G1 IS NONZERO, ADD GG TO THE SOLUTION
C         RETURNED BY THE SUBROUTINE
C
C     -- W(NXDIM, NYDIM, NZDIM) IS UNINITIALIZED
C     -- GG(NXDIM, NYDIM, NZDIM) INITIALIZED TO  G1*HZ*HZ  IN THE
C                                REGION, WITH ARBITRARY VALUES OUTSIDE
C          FOR  I=1, . ,NNX,  J=1,   ,NNY, AND  K=1,  . ,NNZ,
C          GG(I,J,K) CORRESPONDS TO G1((I-1)*HX,(J-1)*HY,(K-1)*HZ)*HZ**2
C          IF  MODE = 1, 3 OR 5,  G1  MAY BE A DUMMY ARRAY (I.E.,
C          IT NEED NOT BE DIMENSIONED BY THE CALLING PROGRAM).
C
C     -- IPP1 IS THE NUMBER OF IRREGULAR POINTS WITH AT LEAST 1
C             INTERIOR NEIGHBOR IN EACH DIRECTION X, Y, AND Z.
C     -- IPP2 IS THE NUMBER OF IRREGULAR POINTS WHICH, ALONG
C             AT LEAST ONE DIRECTION, HAVE TWO EXTERIOR NEIGHBORS.
C
C        IN THE EXCEPTIONAL CASE WHEN  IPP1+IPP2 EQ 0,  THE ROUTINE
C        WILL SOLVE THE PROBLEM ON THE WHOLE CUBE WITH THE
C        BOUNDARY CONDITIONS#
C              G1(X,Y,Z) = 0    Z  LT  0    OR Z  GT  1
C              W(0,Y,Z) = W(1,Y,Z)   AND  W(X,0,Z) = W(X,1,Z)
C              W(X,Y,0)=0 AND W(X,Y,Z) BOUNDED FOR ALL Z
C        ARRAY  GG  MUST BE INITIALIZED TO  G1*HZ*HZ  AND  MODE = 2.
C        W  MAY BE A DUMMY ARRAY  THE ANSWER WILL BE STORED
C        IN THE ARRAY  GG  IN THIS CASE.
C
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C     -- DELTA(3, NIPDIM)  RECORDS + OR - DISTANCE TO BOUNDARY
C             FROM IRREGULAR POINT  L  IN THE  X,  Y,  AND  Z
C             DIRECTIONS  (3*IPP1 + 6*IPP2  VALUES).  THESE DISTANCES
C             ARE EXPRESSED AS MULTIPLES OF THE MESH SPACING  I E.,
C             IF A  DELTA  HAS THE VALUE  Q,  THE DISTANCE IS  Q*H.
C         THERE ARE THREE DELTAS FOR EACH OF THE  IPP1  POINTS
C         FOR  L=1, IPP1,
C          DELTA(1,L) = SHORTER DISTANCE TO BOUNDARY ALONG X DIRECTION
C          DELTA(2,L) = SHORTER DISTANCE TO BOUNDARY ALONG Y DIRECTION
C          DELTA(3,L) = SHORTER DISTANCE TO BOUNDARY ALONG Z DIRECTION
C         THERE ARE SIX DELTAS FOR EACH OF THE IPP2 POINTS,
C         FOR  L=1, IPP2  ,  LL=IPP1+2*L-1,
C          DELTA(1,LL)  AND  DELTA(1,LL+1)  ARE THE DISTANCES TO THE
C             BOUNDARY ALONG THE POSITIVE AND NEGATIVE  X  DIRECTIONS
C          DELTA(2,LL)  AND  DELTA(2,LL+1)  ARE THE DISTANCES TO THE
C             BOUNDARY ALONG THE POSITIVE AND NEGATIVE  Y  DIRECTIONS
C          DELTA(3,LL)  AND  DELTA(3,LL+1)  ARE THE DISTANCES TO THE
C             BOUNDARY ALONG THE POSITIVE AND NEGATIVE  Z  DIRECTIONS
C         THE PROGRAM WILL INTERCHANGE  DELTAS  IF NECESSARY SO THAT
C         FOR  L=1, IPP2  ,  LL=IPP1+2*L-1,
C         ABS(DELTA(S,LL))  LE  ABS(DELTA(S,LL+1))
C         NO  DELTA  CAN BE SO CLOSE TO  0  AS TO CAUSE OVERFLOW
C         UPON DIVISION BY A PRODUCT OF TWO  DELTAS  SUCH SMALL
C         DELTAS  SHOULD BE AVOIDED BY CHANGING THE REGION
C         SLIGHTLY OR BY SHIFTING IT INSIDE THE CUBE OR BY
C         USING ANOTHER MESH SIZE
C
C     -- NNX, NNY, NNZ ARE THE NUMBER OF MESH POINTS IN THE X, Y, AND Z
C                    DIRECTIONS
C        MAX(NNX,NNY) MUST BE  LE  256 UNLESS THE ERROR CHECK IN
C        HELMCK AND THE DIMENSIONS OF IB AND S IN COMMON FFT
C        (SUBROUTINES CUBE,RFORT AND FORT) ARE CHANGED
C         THE MESH SPACINGS WILL BE CALCULATED TO BE
C                 HX = 1 / NNX
C                 HY = 1 / NNY
C                 HZ = 1 / (NNZ - 1)
C         NNX  AND  NNY  MUST BE POWERS OF  2  AND  GE  8  UNLESS
C         THE FFT ROUTINES  RFORT  AND  FORT  ARE REPLACED
C
C     -- NIPDIM, THE DIMENSION OF THE ONE DIMENSIONAL ARRAYS,
C              MUST BE  GE  IPP1+2*IPP2
C     -- NAPDIM , THE DIMENSION OF  AP , MUST
C              BE  GE   MAX(IPP1+2*IPP2, NNX*NNZ, NNY*NNZ )
C     -- ICOORD(3,NIPDIM)  RECORDS THE  3*(IPP1+IPP2)  INDICES OF
C              THE IRREGULAR POINTS.  THESE INDICES MUST LIE BETWEEN
C              2 AND NN-1 INCLUSIVE
C              FOR  L = 1,  IPP1
C                THE  L-TH  COLUMN OF  ICOORD
C                GIVES THE INDICES CORRESPONDING
C                TO DATA IN THE  L-TH  COLUMNS OF
C                DELTA,  P,  R,  AND  AP
C             FOR  L = 1,  IPP2 ,    LL = IPP1 + 2 * L - 1
C                THE  (IPP1+L)-TH  COLUMN OF  ICOORD
C                GIVES THE INDICES CORRESPONDING TO
C                DATA IN THE  LL-TH  AND  (LL+1)-TH
C                COLUMNS OF  DELTA,  P,  R,  AND  AP
C     -- INDORD (NIPDIM)  IS UNINITIALIZED  THE PROGRAM WILL
C              RECORD A CODE (1-6) FOR THE ORDER OF THE DELTAS
C     -- CC  IS THE CONSTANT IN THE HELMHOLTZ EQUATION
C     -- NIT IS THE MAXIMUM NUMBER OF CONJUGATE GRADIENT ITERATIONS
C              ALLOWED.
C     -- EPS IS THE TOLERANCE FOR THE EUCLIDEAN NORM OF
C              THE CAPACITANCE EQUATION RESIDUAL DIVIDED BY THE
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C              SQRT OF THE DIMENSION OF THIS VECTOR
C                          T T      T                 T
C              RESIDUAL = C U F - C C S  WHERE C = U AGV .
C              IT IS DIFFICULT TO GIVE A RELIABLE RULE OF
C              THUMB FOR THE CHOICE OF EPS  FOR MANY PROBLEMS
C              ONE TENTH OF THE DESIRED ACCURACY FOR THE
C              SOLUTION OF THE ORIGINAL DISCRETE PROBLEM IS A
C              SUITABLE VALUE A SMALLER TOLERANCE IS REQUIRED
C              WHEN THE DISCRETE HELMHOLTZ OPERATOR IS CLOSE
C              TO SINGULAR
C    -- S , P , R  ARE OF DIMENSION  NIPDIM
C           AP  IS OF DIMENSION  NAPDIM
C              S IS UNINITIALIZED IF  MODE = 1 OR 2
C              IF MODE  LT  5 , FOR  L=1,IPP1+2*IPP2,
C               R(L) = F(X+DELTA(1,L)*HX, Y, Z)
C               P(L) = F(X, Y+DELTA(2,L)*HY, Z)
C               AP(L) = F(X, Y, Z+DELTA(3,L)*HZ)
C        WHERE X,Y, AND Z ARE THE COORDINATES OF THE
C        IRREGULAR POINT  CORRESPONDING TO THE DELTAS
C        THE VALUES OF  R , P , AND  AP  ARE NOT USED IN THE
C        COMPUTATION IF THE ABSOLUTE VALUE OF THE CORRESPONDING
C        DELTA  IS GREATER THAN 1
C
C    -- IER IS UNINITIALIZED   THE PROGRAM WILL RECORD AN ERROR
C        CODE (0-3)
C        THE USE OF DISCRETE DIPOLES IMPOSES A MILD RESTRICTION
C        ON THE GEOMETRY OF THE REGION   THE THREE MESH POINTS, OBTAINED
C        BY STEPPING FROM AN IRREGULAR POINT IN THE DIRECTION OF THE
C        SMALLEST MAGNITUDE  DELTA,  FROM THIS NEW POINT IN
C        THE DIRECTION OF THE MEDIUM, AND FROM THERE IN THE DIRECTION
C        OF THE LARGEST MUST NOT BE INTERIOR POINTS OF THE REGION
C        ASSOCIATED WITH AN IRREGULAR POINT WHICH HAS AT
C        LEAST  2  EXTERIOR NEIGHBORS IN SOME MESH
C        DIRECTION ARE TWO COLUMNS OF THE ARRAY  DELTA
C        THE  DELTA'S  RELEVANT TO THIS TEST ARE THE
C        SMALLER IN MAGNITUDE OF THE TWO POSSIBLE
C        CHOICES IN EACH COORDINATE DIRECTION   IF THE
C        RESTRICTION IS VIOLATED, A SUBROUTINE  HELMCK  WILL RETURN AN
C        ERROR FLAG  IER = 2   A REFINEMENT OF THE MESH OR
C        A SLIGHT SHIFT OF THE REGION IN THE UNIT CUBE MIGHT
C        RESOLVE THE PROBLEM
C
C   ON OUTPUT
C           W  WILL CONTAIN VALUES OF THE SOLUTION INSIDE THE
C                 REGION AND USELESS VALUES OUTSIDE AND ON THE
C                 BOUNDARY
C          S  WILL RECORD DIPOLE STRENGTHS   THIS IS THE SOLUTION
C                 VECTOR OF THE CAPACITANCE MATRIX EQUATION
C          R  WILL BE THE RESIDUAL OF THE CAPACITANCE EQUATION
C
C          P , AP , AND  GG  WILL BE CHANGED, AND THE  DELTAS  MAY
C          BE REORDERED AS INDICATED ABOVE
C
C        ERROR RETURNS
C            IER=0       NO ERROR
C               =1       ERROR IN INTEGER PARAMETER
C               =2       ERROR IN  ICOORD  OR VIOLATION OF DIPOLE
C                        RESTRICTION OR IRREGULAR POINT MISSING
C               =3       TOO MANY CONJUGATE GRADIENT ITERATIONS
C                        WITHOUT CONVERGENCE  ANSWER DOES NOT
C                        HAVE THE REQUESTED ACCURACY.
C
C
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C       AFTER EACH ITERATION, THE FOLLOWING INFORMATION IS PRINTED
C          -- THE CONJUGATE GRADIENT PARAMETERS  ALPHA  AND  BETA
C               THIS INFORMATION COULD BE USED TO ESTIMATE THE
C               CONDITION NUMBER OF THE CAPACITANCE MATRIX
C          -- THE EUCLIDEAN NORM OF THE RESIDUAL OF THE
C             CAPACITANCE MATRIX EQUATION
C                                  T 1   T             T
C                THE RESIDUAL=C U F-C CS  WHERE C= U AGV
C
C   THE ROLES OF THE SUBROUTINES
C         HELM3D  CONTROLS THE CONJUGATE GRADIENT ITERATION.
C         HELMCK  CHECKS THE INPUT DATA FOR CORRECTNESS
C         VMULT   USES THE DIPOLE STRENGTHS IN A  NIPDIM  ARRAY TO
C                 SET UP THE DIPOLES IN A 3 DIMENSIONAL ARRAY
C                 THIS SUBROUTINE THUS DEFINES A LINEAR MAPPING
C                 FROM A SPACE OF  1-DIMENSIONAL ARRAYS TO A SPACE
C                 OF  3-DIMENSIONAL ARRAYS
C         VTRANS  DEFINES THE TRANSPOSE OF THE MAPPING DEFINED
C                 BY  VMULT
C         UTAMLT  MAPS  3-DIMENSIONAL ARRAYS INTO  1-DIMENSIONAL
C                 ARRAYS BY USING A FINITE DIFFERENCE FORMULA WHICH
C                 CORRESPONDS TO A PART OF THE SHORTLEY-WELLER
C                 APPROXIMATION.  THE REMAINING PART IS HANDLED BY
C                 BNDRY
C         UTATRN  DEFINES THE TRANSPOSE OF THE MAPPING DEFINED BY
C                 UTAMLT
C         BNDRY   PROCESSES THE DIRICHLET DATA AND THE VALUES OF  G1
C                 CLOSE TO THE BOUNDARY, PRODUCING  U(TRANSPOSE)F  FOR
C                 USE IN THE RIGHT HAND SIDE OF THE CAPACITANCE EQUATION
C         CUBE    SOLVES THE HELMHOLTZ EQUATION OVER A CUBE USING A
C                 FOURIER-TOEPLITZ ALGORITHM
C         RFORT   IS A FAST FOURIER TRANSFORM ROUTINE DUE TO
C                 W PROSKUROWSKI WHO REVISED A CODE WRITTEN BY J COOLEY
C                 IT IS USED BY SUBROUTINE CUBE
C         FORT    IS A SUBROUTINE CALLED BY  RFORT
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