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

DIANNE P. O'LEARY
University of Maryland
and
OLOF WIDLUND
New York University

Key Words and Phrases: Helmholtz equation, capacitance matrix, fast Poisson solvers, conjugate gradients
CR Categories: 5.17
Language FORTRAN

DESCRIPTION
This algorithm provides an approximate solution to the Helmholtz equation
\[-\Delta u + cu = g \quad \text{in } \Omega\]
with a Dirichlet boundary condition
\[u = f \quad \text{on } \Gamma, \text{ the boundary of } \Omega.\]

Here \(\Omega\), 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 \(\Delta\) 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 method.
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 $\Omega$ 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 $\Omega$ and are near the boundary $\Gamma$. 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 $\Gamma$. 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 $N_X$, $N_Y$, and $N_Z$ be the numbers of mesh points in the cube along the three coordinate axes, where $N_X$ and $N_Y$ are powers of 2. We denote the number of mesh points in $\Omega$ with at least one of their six nearest neighbors on or outside the boundary $\Gamma$ by $IPP_1 + IPP_2$, where $IPP_2$ 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 $IPP_1 + IPP_2$ 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 $\Gamma$, and the value of the function $g$ at mesh points in $\Omega$. 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 $N_X \times N_Y \times N_Z$ (one if $g = 0$), four integer and six real arrays of dimension $IPP_1 + 2 \times IPP_2$, and one real array of dimension $\max(IPP_1 + 2 \times IPP_2, N_X \times N_Z, N_Y \times N_Z)$. Each conjugate gradient iteration requires time proportional to $N_X \times N_Y \times N_Z \times \log(N_X \times N_Y)$, 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 $32 \times 32 \times 24$ 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 $0.55 \times 10^{-3}$ 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


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, 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, NAPDIM, ICOORD, INDORD(NIPDIM), CC
REAL W(NXDIM, NYDIM, NZDIM), GG(NXDIM, NYDIM, NZDIM), DELTA(3, NIPDIM), CC, EPS, S(NIPDIM), R(NIPDIM), P(NIPDIM), AP(NAPDIM)

THIS PROGRAM WAS DEVELOPED BY DIANNE O'LEARY AND OLOF WIDLUND
THIS IS VERSION MD2, OCTOBER, 1979

THIS PROGRAM SOLVES THE DIRICHLET PROBLEM FOR THE HELMHOLTZ EQUATION OVER A GENERAL BOUNDED 3 DIMENSIONAL REGION IMBEDDED IN A UNIT CUBE

- W - W - W + CC*W = G1 IN THE REGION
  XX YY ZZ

W = F ON THE BOUNDARY


REFERENCES

MATH COMP 33, 1979 849-880

PROSKUROWSKI AND WIDLUND, MATH COMP 30, 1976 443-469.
ALSO NYU-DOE REPORT
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PROSKUROWSKI, LAWRENCE BERKELEY LAB REPORTS AND
"NUMERICAL SOLUTION OF HELMHOLTZ’S EQUATION BY
IMPLICIT CAPACITANCE MATRIX METHODS," ACM TRANS
ON MATH SOFTWARE 5, 1979 36-49.

SHIEH, MRC-WISCONSIN REPORTS AND NUMER. MATH 29
1978 307-327

MACHINE DEPENDENT FEATURES

THIS PROGRAM SHOULD BE CONVERTED TO DOUBLE PRECISION
IF IT IS TO BE USED ON COMPUTERS WITH SHORT WORD
LENGTH, SUCH AS IBM 360/370

GENERAL DESCRIPTION OF THE PARAMETERS:

INTEGER VALUES
- DIMENSIONS OF ARRAYS (NXDIM, NYDIM, NZDIM,
  NIPDIM, NAPDIM)
- NUMBER OF MESH POINTS IN CUBE (NNX X NNY X
  NNZ)
- NUMBER OF POINTS IN REGION ADJACENT TO BOUNDARY
  (IPPI, IPP2)
- MAXIMUM NUMBER OF ITERATIONS ALLOWED (NIT)
- ERROR CODE (IER)
- CODE TO CONTROL PROGRAM OPTIONS (MODE)

REAL VALUES
- HELMHOLTZ CONSTANT (CC)
- CONVERGENCE TOLERANCE (EPS)

INTEGER ARRAYS
- COORDINATES OF POINTS IN REGION ADJACENT TO
  BOUNDARY ('IRREGULAR POINTS') (ICOORD)
- WORK SPACE (INDORD)

REAL ARRAYS
- GI VALUES (GG)
- BOUNDARY VALUES (R, P, AP)
- DISTANCES FROM IRREGULAR POINTS TO BOUNDARY
  (DELTA)
- WORK SPACE (W, S)

TOTAL ARRAY SPACE NEEDED
- REAL 2 NXdIM * NYDIM * NZDIM (1 IF GI=0)
- 6 NIPDIM
- 1 NAPDIM
- INTEGER
- 4 NIPDIM

WHERE NXdIM GE NNX, NYDIM GE NNY,
  NZDIM GE NNZ,
  NIPDIM GE IPPI + 2 * IPP2,
  NAPDIM GE MAX (IPPI+2*IPP2, NNX*NNZ,
  NNY*NNZ)
IN THIS DOCUMENTATION, \( NN \) REFERS TO \( NNX, NNY, \) OR \( NNZ \)
AS APPROPRIATE, AND SIMILARLY \( H \) REFERS TO \( HX, HY, \) OR \( HZ \).
The mesh point \((X,Y,Z)\) is said to have 6 neighbors:
\((X+HX,Y,Z), (X-HX,Y,Z), (X,Y+HY,Z), (X,Y-HY,Z),
(X,Y,Z+HZ), \) AND \((X,Y,Z-HZ)\).
A mesh point is called irregular if it is in the interior of
the region and at least one of its six neighbors is on or
outside the boundary.

**NOTE**

**ON INPUT**

--- **MODE** = 1 IF THE REGION HAS BEEN CHANGED FROM THE PREVIOUS CALL
AND \( G1=0 \)
--- 2 IF THE REGION HAS BEEN CHANGED FROM THE PREVIOUS CALL
AND \( G1 \) IS NONZERO
--- 3 IF THE REGION IS THE SAME AS ON THE PREVIOUS CALL
AND \( G1=0 \)
--- 4 IF THE REGION IS THE SAME AS ON THE PREVIOUS CALL
AND \( G1 \) IS NONZERO
--- 5 IF THE PROBLEM IS THE SAME AS ON THE PREVIOUS CALL,
\( G1=0 \), AND THE ONLY CHANGE IS THAT \( EPS \) AND/OR \( NIT \)
MAY HAVE BEEN CHANGED
--- 6 IF THE PROBLEM IS THE SAME AS ON THE PREVIOUS CALL,
\( G1 \) IS NONZERO, AND THE ONLY CHANGE IS THAT \( EPS \)
AND/OR \( NIT \) MAY HAVE BEEN CHANGED

IF **MODE** = 3, 4, 5, OR 6 \( DELTA, ICOORD, INDORD, NXdIM, \)
**NYDIM, NZDIM, NNX, NNY, NNZ, IPP1, AND IPP2** MUST BE
UNCHANGED FROM THE PREVIOUS CALL THE CURRENT VALUE OF \( S \)
WILL BE USED AS THE INITIAL GUESS FOR THE DIPOLE STRENGTHS
\( (S=0 \) WILL BE USED IF **MODE**=1 OR 2 \)
TO IMPROVE THE ACCURACY OF A PREVIOUSLY CALCULATED SOLUTION,
USE **MODE**=5 OR **MODE**=6 IF ROUNDOFF IS NOT SUSPECTED. IF
ROUNDOFF IS SUSPECTED, REINITIALIZE THE BOUNDARY VALUES IN \( R, \)
\( AP \), AND \( P \), AND USE **MODE** = 3 TO FORCE THE RESIDUAL TO BE
RECOMPUTED, IF \( G1 \) IS NONZERO, ADD \( GG \) TO THE SOLUTION
RETURNED BY THE SUBROUTINE

--- **W**(**NXDIM, NYDIM, NZDIM**) IS UNINITIALIZED
--- **GG**(**NXDIM, NYDIM, NZDIM**) INITIALIZED TO \( G1*HZ*HZ \) IN THE
REGION, WITH ARBITRARY VALUES OUTSIDE
FOR I=1, \( ..., NNX, \) J=1, \( ..., NNY, \) AND K=1, \( ..., NNZ, \)
**GG**(I,J,K) CORRESPONDS TO \( G1((I-1)*HX,(J-1)*HY,(K-1)*HZ)*HZ**2 \)
IF **MODE** = 1, 3 OR 5, \( G1 \) MAY BE A DUMMY ARRAY (I.E.,
IT NEED NOT BE DIMENSIONED BY THE CALLING PROGRAM).

--- **IPP1** IS THE NUMBER OF IRREGULAR POINTS WITH AT LEAST 1
INTERIOR NEIGHBOR IN EACH DIRECTION \( X, Y, \) AND \( Z \).
--- **IPP2** IS THE NUMBER OF IRREGULAR POINTS WHICH, ALONG
AT LEAST ONE DIRECTION, HAVE TWO EXTERIOR NEIGHBORS.

IN THE EXCEPTIONAL CASE WHEN **IPP1**+**IPP2** EQ 0, THE ROUTINE
WILL SOLVE THE PROBLEM ON THE WHOLE CUBE WITH THE
BOUNDARY CONDITIONS:
\( G1(X,Y,Z) = 0 \) \( Z \) LT 0 OR \( Z \) GT 1
\( W(0,Y,Z) = W(1,Y,Z) \) AND \( W(X,0,Z) = W(X,1,Z) \)
\( W(X,Y,0) = 0 \) AND \( W(X,Y,Z) \) BOUNDED FOR ALL \( Z \)
**ARRAY** **GG** MUST BE INITIALIZED TO \( G1*HZ*HZ \) AND **MODE** = 2.
**W** MAY BE A DUMMY ARRAY THE ANSWER WILL BE STORED
IN THE **ARRAY** **GG** IN THIS CASE.
-- DELTA(3, NIPDIM) RECORDS + OR - DISTANCE TO BOUNDARY
THERE ARE THREE DELTAS FOR EACH OF THE IPP1 POINTS, FOR L=1, IPP1.
DELTA(1, L) = SHORTER DISTANCE TO BOUNDARY ALONG X DIRECTION
DELTA(2, L) = SHORTER DISTANCE TO BOUNDARY ALONG Y DIRECTION
DELTA(3, L) = SHORTER DISTANCE TO BOUNDARY ALONG Z DIRECTION
THERE ARE SIX DELTAS FOR EACH OF THE IPP2 POINTS, FOR L=1, IPP2, LL=IPP1+2*L-1,
DELTA(1, LL) AND DELTA(1, LL+1) ARE THE DISTANCES TO THE BOUNDARY ALONG THE POSITIVE AND NEGATIVE X DIRECTIONS
DELTA(2, LL) AND DELTA(2, LL+1) ARE THE DISTANCES TO THE BOUNDARY ALONG THE POSITIVE AND NEGATIVE Y DIRECTIONS
DELTA(3, LL) AND DELTA(3, LL+1) ARE THE DISTANCES TO THE BOUNDARY ALONG THE POSITIVE AND NEGATIVE Z DIRECTIONS
THE PROGRAM WILL INTERCHANGE DELTAS IF NECESSARY SO THAT FOR L=1, IPP2, LL=IPP1+2*L-1,
ABS(DELTA(S, LL)) LE ABS(DELTA(S, LL+1))
NO DELTA CAN BE SO CLOSE TO 0 AS TO CAUSE OVERFLOW UPON DIVISION BY A PRODUCT OF TWO DELTAS SUCH SMALL DELTAS SHOULD BE AVOIDED BY CHANGING THE REGION SLIGHTLY OR BY SHIFTING IT INSIDE THE CUBE OR BY USING ANOTHER MESH SIZE.

-- NNX, NNY, NNZ ARE THE NUMBER OF MESH POINTS IN THE X, Y, AND Z DIRECTIONS
MAX(NNX, NNY) MUST BE LE 256 UNLESS THE ERROR CHECK IN HELMCK AND THE DIMENSIONS OF IB AND S IN COMMON FFT (SUBROUTINES CUBE, RFORT AND FORT) ARE CHANGED
THE MESH SPACINGS WILL BE CALCULATED TO BE
HX = 1 / NNX
HY = 1 / NNY
HZ = 1 / (NNZ - 1)
NNX AND NNY MUST BE POWERS OF 2 AND GE 8 UNLESS THE FFT ROUTINES RFORT AND FORT ARE REPLACED

-- NIPDIM, THE DIMENSION OF THE ONE DIMENSIONAL ARRAYS, MUST BE GE IPP1+2*IPP2
-- NAPDIM, THE DIMENSION OF AP, MUST BE GE MAX(IPP1+2*IPP2, NNX*NNZ, NNY*NNZ)
-- ICOORD(3, NIPDIM) RECORDS THE 3*(IPP1+IPP2) INDICES OF THE IRREGULAR POINTS. THESE INDICES MUST LIE BETWEEN 2 AND NN-1 INCLUSIVE
FOR L = 1, IPP1
THE L-TH COLUMN OF ICOORD GIVES THE INDICES CORRESPONDING TO DATA IN THE L-TH COLUMNS OF DELTA, P, R, AND AP
FOR L = 1, IPP2, LL = IPP1 + 2 * L - 1
THE (IPP1+L)-TH COLUMN OF ICOORD GIVES THE INDICES CORRESPONDING TO DATA IN THE LL-TH AND (LL+1)-TH COLUMNS OF DELTA, P, R, AND AP
-- INDORD (NIPDIM) IS UNINITIALIZED THE PROGRAM WILL RECORD A CODE (1-6) FOR THE ORDER OF THE DELTAS
-- CC IS THE CONSTANT IN THE HELMHOLTZ EQUATION
-- NIT IS THE MAXIMUM NUMBER OF CONJUGATE GRADIENT ITERATIONS ALLOWED
-- EPS IS THE TOLERANCE FOR THE EUCLIDEAN NORM OF THE CAPACITANCE EQUATION RESIDUAL DIVIDED BY THE
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SQRT OF THE DIMENSION OF THIS VECTOR

RESIDUAL = C U F - C C S WHERE C = U A G V .

IT IS DIFFICULT TO GIVE A RELIABLE RULE OF
THUMB FOR THE CHOICE OF EPS FOR MANY PROBLEMS
ONE TENTH OF THE DESIRED ACCURACY FOR THE
SOLUTION OF THE ORIGINAL DISCRETE PROBLEM IS A
SUITEABLE VALUE A SMALLER TOLERANCE IS REQUIRED
WHEN THE DISCRETE HELMHOLTZ OPERATOR IS CLOSE
TO SINGULAR

-- S , P , R ARE OF DIMENSION NIPDIM
AP IS OF DIMENSION NAPDIM
S IS UNINITIALIZED IF MODE = 1 OR 2
IF MODE LT 5 , FOR L=1.IPP1+2*IPP2,
R(L) = F(X+DELTA(1,L)*HX, Y, Z)
P(L) = F(X, Y+DELTA(2,L)*HY, Z)
AP(L) = F(X, Y, Z+DELTA(3,L)*HZ)
WHERE X, Y, AND Z ARE THE COORDINATES OF THE
IRREGULAR POINT CORRESPONDING TO THE DELTAS
THE VALUES OF R , P , AND AP ARE NOT USED IN THE
COMPUTATION IF THE ABSOLUTE VALUE OF THE CORRESPONDING
DELTA IS GREATER THAN 1

-- IER IS UNINITIALIZED THE PROGRAM WILL RECORD AN ERROR
CODE (0-3)
THE USE OF DISCRETE DIPOLES IMPOSES A MILD RESTRICTION
ON THE GEOMETRY OF THE REGION THE THREE MESH POINTS, OBTAINED
BY STEPPING FROM AN IRREGULAR POINT IN THE DIRECTION OF THE
SMALLEST MAGNITUDE DELTA, FROM THIS NEW POINT IN
THE DIRECTION OF THE MEDIUM, AND FROM THERE IN THE DIRECTION
OF THE LARGEST MUST NOT BE INTERIOR POINTS OF THE REGION
ASSOCIATED WITH AN IRREGULAR POINT WHICH HAS AT
LEAST 2 EXTERIOR NEIGHBORS IN SOME MESH
DIRECTION ARE TWO COLUMNS OF THE ARRAY DELTA
THE DELTA'S RELEVANT TO THIS TEST ARE THE
SMALLER IN MAGNITUDE OF THE TWO POSSIBLE
CHOICES IN EACH COORDINATE DIRECTION IF THE
RESTRICTION IS VIOLATED, A SUBROUTINE HELMCK WILL RETURN AN
ERROR FLAG IER = 2 A REFINEMENT OF THE MESH OR
A SLIGHT SHIFT OF THE REGION IN THE UNIT CUBE MIGHT
RESOLVE THE PROBLEM

ON OUTPUT
W WILL CONTAIN VALUES OF THE SOLUTION INSIDE THE
REGION AND USELESS VALUES OUTSIDE AND ON THE
BOUNDARY
S WILL RECORD DIPOLE STRENGTHS THIS IS THE SOLUTION
VECTOR OF THE CAPACITANCE MATRIX EQUATION
R WILL BE THE RESIDUAL OF THE CAPACITANCE EQUATION
P , AP , AND Gg WILL BE CHANGED, AND THE DELTAS MAY
BE REORDERED AS INDICATED ABOVE

ERROR RETURNS
IER=0 NO ERROR
=1 ERROR IN INTEGER PARAMETER
=2 ERROR IN ICOORD OR VIOLATION OF DIPOLE
RESTRICTION OR IRREGULAR POINT MISSING
=3 TOO MANY CONJUGATE GRADIENT ITERATIONS
WITHOUT CONVERGENCE ANSWER DOES NOT
HAVE THE REQUESTED ACCURACY.
AFTER EACH ITERATION, THE FOLLOWING INFORMATION IS PRINTED
-- THE CONJUGATE GRADIENT PARAMETERS ALPHA AND BETA
THIS INFORMATION COULD BE USED TO ESTIMATE THE
CONDITION NUMBER OF THE CAPACITANCE MATRIX
-- THE EUCLIDEAN NORM OF THE RESIDUAL OF THE
CAPACITANCE MATRIX EQUATION
\[
\| r \|_2 = \left( \sum_{i=1}^{n} (r_i)^2 \right)^{1/2}
\]
THE RESIDUAL = \( C(U^T F - C) \) WHERE \( C := U \cdot A \cdot C \)

THE ROLES OF THE SUBROUTINES

HELM3D CONTROLS THE CONJUGATE GRADIENT ITERATION.
HELMCK CHECKS THE INPUT DATA FOR CORRECTNESS
VMULT USES THE DIPOLE STRENGTHS IN A NIPDIM ARRAY TO
SET UP THE DIPOLES IN A 3 DIMENSIONAL ARRAY
THIS SUBROUTINE THUS DEFINES A LINEAR MAPPING
FROM A SPACE OF 1-DIMENSIONAL ARRAYS TO A SPACE
OF 3-DIMENSIONAL ARRAYS
VTRANS DEFINES THE TRANPOSE OF THE MAPPING DEFINED
BY VMULT
UTAMLT MAPS 3-DIMENSIONAL ARRAYS INTO 1-DIMENSIONAL
ARRAYS BY USING A FINITE DIFFERENCE FORMULA WHICH
CORRESPONDS TO A PART OF THE SHORTLEY-WELLER
APPROXIMATION. THE REMAINING PART IS HANDLED BY
BDNY
UTATRN DEFINES THE TRANPOSE OF THE MAPPING DEFINED BY
UTAMLT
BDNY PROCESSES THE DIRICHLET DATA AND THE VALUES OF \( g_j \)
CLOSE TO THE BOUNDARY, PRODUCING \( U^T (F - C) \) FOR
USE IN THE RIGHT HAND SIDE OF THE CAPACITANCE EQUATION
CUBE SOLVES THE HELMHOLTZ EQUATION OVER A CUBE USING A
FOURIER-TOEPLITZ ALGORITHM
RFORT IS A FAST FOURIER TRANSFORM ROUTINE DUE TO
W PROSKUROWSKI WHO REVISED A CODE WRITTEN BY J CONLEY
IT IS USED BY SUBROUTINE CUBE
FORT IS A SUBROUTINE CALLED BY RFORT