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ELLPACK User's Guide Supplement

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ELLPACK USER'S GUIDE SUPPLEMENT

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May 1, 1981
CSD-TR 363

ABSTRACT

This report is a supplement to CSD-TR 289: ELLPACK 77 USER'S GUIDE. It describes the ELLPACK system as of Spring 1981 and its main purpose is to identify and document the new modules available in the ELLPACK system as of this date. The ELLPACK language is being revised with the ELLPACK 77 and ELLPACK 78 features merged and a completely new implementation is well under way. It is expected to be operational in 1981.

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1. GENERAL REMARKS

This report is a supplement to the report

ELLPACK 77 USER'S GUIDE
CSD-TR 289, September 15, 1978
Revised July 1, 1980

The primary reason for the revision was to describe new problem solving modules that had been added to the ELLPACK system. That is also the primary reason for this supplement, the ELLPACK version of April, 1981 is described. Three completely new modules (FISHPAK-HELMHOLTZ, P3CL COLLORDER and YALE GALERKIN) have been added and significant new capabilities have been added to NESTED DISSECTION and the ITPACK modules. A few other notes on the modules are given (including all those added in the July 1, 1980 revision) and some miscellaneous errata given.

The principal "general" change in the April, 1981 version of ELLPACK is that the local quadratic polynomial interpolation algorithm to define U globally for finite difference methods have been replaced by a spline interpolant whose polynomial degree is chosen to be compatible with the order of the discretization method. Thus quadratic interpolation with its $O(h^3)$ local error is reasonable for ordinary finite differences, but not for a higher order method of discretization. The algorithm uses the tensor product B-spline programs of Carl deBoor and were put into ELLPACK by Ronald Boisvert.

A substantial price is paid for this better interpolation as the interpolant requires memory proportional to the number of unknowns. The factor of proportionality depends on the degree, starting at 3 for cubic splines. Memory is a scarce resource in many applications of ELLPACK and it is planned to have the choice of interpolation method optional in future versions so those who do not need better interpolation will not have memory allocated for it.

Miscellaneous errata for CSD-TR 289 (Revised) follows

Page:

11 (bottom) The example boundary conditions are wrong, the last 3 lines should be

\[
Y = -1., \text{ MIXED } = (B(X,Y,2,1))U \quad (B(X,Y,2,2)UY = B(X,Y,2,4) \\
X = 2., \text{ MIXED } = (B(X,Y,3,1))U \quad (B(X,Y,3,3)UX = B(X,Y,3,4) \\
Y = 3., \text{ MIXED } = (B(X,Y,4,1))U \quad (B(X,Y,4,3)UY = B(X,Y,4,4)
\]
The function $F(X,Y)$ may be considerably simplified as ELLPACK now has a standard function $U(X,Y)$ available at all times after a discretization and solution is made. Thus, this program can be replaced by:

```fortran
FUNCTION F(X,Y)
   F = U(X,Y) ** 2 *(X ** 2 + Y ** 2) * EXP(-X * Y)
   RETURN
END
```

To be safe, use $U$ in an OUTPUT module (e.g. OUTPUT. MAX-U) before using $U$ elsewhere.
MODULE NOTES

A. Old (From July 1, 1980 revision)

P3-C1 COLLOCATION: There is a restriction on the grid size as follows:

A. As distributed by IMSL and on the CDC6500, largest grid is 14 x 14
B. As on the Purdue VAX, largest grid is 32 x 32

P3-C1 GALERKIN: There is a restriction on the grid size as follows:

A. As distributed by IMSL and on the CDC6500, largest grid is 14 x 14
B. As on the Purdue VAX, largest grid is 32 x 32

FFT9-POINT: The following limitations apply

A. IORDER=2 must have HX = HY
B. IORDER=4 or 6, must have lower left corner of domain = (0,0)

SPARSE GE-PIVOTING: This module cannot follow RED-BLACK

YALE SPARSE: NSP is computed by default if not specified here or by YALE MIN DEG. If NSP is specified by more than one YALE module, the largest value is used. The default value is usually way too large for small systems and is sometimes too small for large ones.

YALE ENVELOPE: See YALE SPARSE note

B. New

2DEPEN: The name has been changed to P2CO-TRIANGLES. This is not the same software as sold by IMSL with the name 2DEPEN.

ITPACK: Version 2A is included, this version is applicable to non-symmetric problems. The methods have not been changed, but if a linear system is "nearly" symmetric then the methods are frequently still very effective.

A new parameter is included. ITPINT = .FALSE. asks ITPACK to use a default initialization, ITPINT = .TRUE. specifies that the user has initialized the unknowns and the default is to be skipped.

YALE SPARSE: This module assumes that any indexing done is symmetric (the same permutations are applied to the rows and columns of the matrix). In particular, YALE SPARSE cannot follow P3-C1 COLLORDER.

YALE ENVELOPE: See YALE SPARSE note.
NESTED DISSECTION: This indexing is now available for three dimensional problems. The possible values for the parameter are:

<table>
<thead>
<tr>
<th>NTYPE</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>5 point nested dissection (2 DIM)</td>
</tr>
<tr>
<td>9</td>
<td>9 point nested dissection (2 DIM)</td>
</tr>
<tr>
<td>7</td>
<td>7 point nested dissection (3 DIM)</td>
</tr>
<tr>
<td>27</td>
<td>27 point nested dissection (3 DIM)</td>
</tr>
</tbody>
</table>
ELLPACK MODULES

All the ELLPACK modules are described in CSD-TR 289 (Revised July, 1980) or here. The modules are listed below, the numbers provide a simple designation of ELLPACK programs.

<table>
<thead>
<tr>
<th>Discretization</th>
<th>Indexing</th>
<th>Solution</th>
</tr>
</thead>
<tbody>
<tr>
<td>1. 5-POINT STAR</td>
<td>14. NATURAL</td>
<td>20. LINPACK BAND</td>
</tr>
<tr>
<td>2. 7-POINT 3D</td>
<td>15. RED-BLACK</td>
<td>21. LINPACK SPD BAND</td>
</tr>
<tr>
<td>3. PC-C1 COLLOCATION</td>
<td>16. YALE MIN DEG</td>
<td>22. SPARSE GE-PIVOTING</td>
</tr>
<tr>
<td>4. P3-C1 GALERKIN</td>
<td>17. YALE RCM</td>
<td>33. SOR</td>
</tr>
<tr>
<td>5. HODIE-HELMHOLTZ</td>
<td>32. NESTED</td>
<td>34. JACOBI SI</td>
</tr>
<tr>
<td>6. HODIE-ACF</td>
<td>DISSECTION</td>
<td>35. JACOBI CG</td>
</tr>
<tr>
<td>7. HODIE 27-POINT 3D</td>
<td></td>
<td></td>
</tr>
<tr>
<td>9. FFT 9-POINT</td>
<td>41. P3Cl COLLORDER</td>
<td>36. SYMMETRIC SOR SI</td>
</tr>
<tr>
<td>10. P2CO TRIANGLES</td>
<td></td>
<td>37. SYMMETRIC SOR CG</td>
</tr>
<tr>
<td>11. MARCHING ALGORITHM</td>
<td></td>
<td>38. REDUCED SYSTEM SI</td>
</tr>
<tr>
<td>12. DYAKANOV-CG</td>
<td></td>
<td>39. REDUCED SYSTEM CG</td>
</tr>
<tr>
<td>13. DYAKANOV-CG</td>
<td></td>
<td>40. YALE SPARSE</td>
</tr>
<tr>
<td>40. FISHPAK HELMHOLTZ</td>
<td></td>
<td>41. YALE ENVELOPE</td>
</tr>
<tr>
<td>42. YALE GALERKIN</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Modules 18, 19 and 23-24 have been retired, 7 is reserved for HODIE-ACDEF.

Figure A4 shows some of the module sequences which are legal in ELLPACK. Not all legal paths are indicated (3-16-22 will work, 3-16-30 will not) and some combinations might be legal, but fail (3-41-33 gives a divergent iteration). The user should consult the module descriptions for more details and be prepared to experiment with unusual combinations.

<table>
<thead>
<tr>
<th>MODULE</th>
<th>MAY BE FOLLOWED BY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>14, 15, 16, 17, 32</td>
</tr>
<tr>
<td>2</td>
<td>14, 15, 16, 17, 32</td>
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<td>3</td>
<td>14, 41</td>
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<td>4</td>
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<tr>
<td>6</td>
<td>14, 16, 17, 32</td>
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<tr>
<td>8-13, 40</td>
<td>None</td>
</tr>
<tr>
<td>14</td>
<td>20, 21, 22, 30, 31, 33, 34, 35, 36, 37</td>
</tr>
<tr>
<td>15</td>
<td>30, 31, 38, 39</td>
</tr>
<tr>
<td>16</td>
<td>22, 30, 31</td>
</tr>
<tr>
<td>17</td>
<td>22, 30, 31</td>
</tr>
<tr>
<td>32</td>
<td>22, 30, 31</td>
</tr>
<tr>
<td>41</td>
<td>20, 33, 34, 35, 36, 37</td>
</tr>
<tr>
<td>42</td>
<td>14, 16, 17</td>
</tr>
</tbody>
</table>

Figure A4. Module Compatibility Table
MODULE NAME: FISHPAK-HELMHOLTZ

AUTHORS: John Adams, Paul Swarztrauber and Roland Sweet, June 1979
(Modified for use in ELLPACK by Wayne R. Dyksen, September, 1980)

INITIAL-FINAL INTERFACES: Equation Formation - Equation Solution

MODULE FUNCTION: FISHPAK-HELMHOLTZ solves the standard five-point finite
difference approximation to the Helmholtz equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \lambda u = f(x,y)$$

in a rectangle subject to Dirichlet or Neumann boundary conditions on any
side of the rectangle.

RESTRICTIONS ON USE:
Two dimensions
Rectangular domain
Helmholtz equation
Dirichlet or Neumann boundary conditions
Uniform grid, at least 4 x 4

METHOD DESCRIPTION: FISHPAK-HELMHOLTZ invokes the Fishpak routine
HWSCRT which uses the standard five-point difference formula and the fast
Fourier transform to approximate the solution of a Helmholtz equation in a
rectangle with Dirichlet or Neumann boundary conditions on any side.
FISHPAK-HELMHOLTZ is compatible with the June 1979 version of Fishpak
(Version 3).

If Neumann boundary conditions are specified on all four sides of the
rectangle for a Poisson equation ($\lambda=0$), then a solution may not exist. A
constant, PERTRB, is calculated and subtracted from the right side $f$, which
ensures that a solution exists. Fishpak then computes this solution
which is a least squares solution to the original approximation. This solu-
tion plus any constant is also a solution. Hence, the solution is not unique.
The value of PERTRB should be small compared to the right side $f$, other-
wise a solution is obtained to an essentially different problem. This com-
parison should always be made to insure that a meaningful solution has
been obtained. The value of PERTRB is printed if $\text{LEVEL} \geq 2$.

Fishpak will attempt to find a solution even if $\lambda > 0$ in which case a solu-
tion may not exist.

PARAMETERS: None

KEYWORDS: None

PERFORMANCE ESTIMATES: FISHPAK-HELMHOLTZ requires memory for one copy
of the unknowns as well as a workspace of length $4 \cdot \text{NGRIDY} + (13$
$+ \text{INT} (\log_2 (\text{NGRIDX})) \cdot \text{NGRIDX}$. The Execution time is roughly proportional
to $\text{NGRIDX} \cdot \text{NGRIDY} \cdot \log_2 (\text{NGRIDY})$, but also depends on the boundary condi-
tions.
MODULE NAME: P3C1COLLORDER

AUTHOR: Wayne R. Dyksen, January 1981

INITIAL-FINAL INTERFACES: Equation Indexing - Equation Solution

MODULE FUNCTION: P3C1COLLORDER reorders the linear system generated by P3-C1 COLLOCATION so that the reordered system has a non-zero diagonal.

RESTRICTIONS ON USE: P3C1COLLORDER should be used only in conjunction with P3-C1 COLLOCATION. The keyword HOMOGENEOUS should not be used in the boundary segment of the ELLPACK program since P3C1COLLORDER is only designed to work on the linear system generated by the non-homogeneous version of P3-C1 COLLOCATION.

To insure a non-zero diagonal, the coefficient functions in the PDE and the boundary conditions must not vanish. Also, the boundary conditions on any side may include only values of $U$ and/or its normal derivative.

METHOD DESCRIPTION: The grid points are numbered in the natural way from west to east, south to north. The collocation points (equations, rows) are associated with the nearest grid point and are numbered in groups of four in the order of their corresponding grid point. The Hermite bicubic basis functions (unknowns, columns) are ordered in the natural way from west to east, south to north. Some of the basis functions are then reordered depending on the boundary conditions to insure a non-zero diagonal. For complete details with examples see the comments in the routine P3C1NX.

Besides having a non-zero diagonal, the reordered coefficient matrix exhibits other nice properties. It is a band matrix with band width $4(NGRIDX-1)$. It is block symmetric in that it consists of $4\times4$ blocks which if $B_{ij} \neq 0$ then $B_{ji} \neq 0$. There are at most 16 non-zero entries per row occurring in 4 blocks. All the symmetric pairs of off-diagonal blocks can be stored in their natural order within one $4\times4$ block.


PARAMETERS: None

KEYWORDS: None

PERFORMANCE ESTIMATES: P3C1COLLORDER requires no workspace storage.
MODULE NAME: YALE GALERKIN

AUTHOR/DATE: S. C. Eisenstat, M.H. Schultz, and A. Weiser, February 1981

INITIAL/FINAL INTERFACES:
   EQUATION FORMATION/EQUATION INDEXING

MODULE FUNCTION: Discretizes a self-adjoint elliptic operator with
   Dirichlet boundary conditions.

RESTRICTIONS ON USE: Two dimensions, self-adjoint operator, Dirichlet
   boundary conditions.

METHOD DESCRIPTION: Galerkin's method. Basis functions are tensor-product
   B-splines of order K and global continuity NCD. The default
   is smooth bicubic splines (K=4, NCD=2). The boundary
   conditions are imposed via a least squares penalty method.
   Note that
   a) No advantage is taken of homogeneous boundary
      conditions or separable coefficient functions
   b) For non-smooth splines. (NCD<K-1) the natural
      ordering of equations is inappropriate for this
      module.

PARAMETERS: K-order of the B-splines
   (default=4)
NCD - global continuity
   (default=2)

KEYWORDS THAT AFFECT MODULE:
   TWO DIMENSIONS, SELF-ADJOINT,
   DIRICHLET.
MODULE NAME:  H3C) TRIANGLES *

AUTHOR/DATE:  G. Sewell, 10/16/78

INITIAL/FINAL INTERFACE:  EQUATION FORMATION-OUTPUT

RESTRICTIONS:  Two-dimensions, self-adjoint

MODULE DESCRIPTION:  Galerkin's method with 6-node quadratic triangular elements, user-
controlled grading of the triangular mesh, and the frontal method to
organize out-of-core storage of the matrix when necessary.

PARAMETERS:

NTRI- number of triangles desired in final triangulation
MEM- workspace storage = 71*NTRI  if external storage to be used
       46*NTRI + 15*NTRI**1.5 otherwise

The grid is used to define an initial triangulation.  This triangulation
will have about 4 triangles for each grid square which intersects the
region, so NTRI must be larger than this number.  The closure of the
intersection of any grid square with the region must be convex or
nearly so.  Thus it is necessary, in general, that any region corner
with exterior angle less than 180° be cut by a grid line which divides
the exterior angle into two parts.  (In the case of a 90° exterior
angle with edges parallel to the axes, however, it is sufficient to put
a grid point at that corner.)

FORTRAN:

Function D3EST(X,Y) must be user supplied.
The program grades the initial triangulation so that the final
triangulation is most dense where D3EST is largest.  In particular,
it attempts to distribute D3EST(X,Y)*D**3 uniformly, where (X,Y)
is the center of triangle j and D is its diameter.  If D3EST is an
estimate of the function

\[ \max_{i+j=3} \left| \frac{D^3}{Dx^2 + Dy^2} \right| \]

It is possible to obtain optimal order convergence to the solution of
some singular problems.

* This was formerly named 'XDEEP', it is not the software sold by IMSL, under
 that name.
ELLPACK LITERATURE

1976


1977


1978


1979


1980


1981


