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ELLPACK User's Guide Supplement

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ELLPACK USER'S GUIDE SUPPLEMENT

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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.

CONTENTS

1. General Remarks

2. Appendix 3 Update: ELLPACK modules

   Module Notes
   FISHPAK-HELMHOLTZ
   P3C1 COLLORDER
   YALE GALERKIN
   P3CO TRIANGLES

3. ELLPACK Literature

ELLPACK USER'S GUIDE SUPPLEMENT

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, P3C1 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is that the local quadratic polynomial interpolation algorithm to define U globally for finite difference methods have been replaced by a spline interpolant whose polynomial degree is chosen to be compatible with the order of the discretization method.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., MIXED = (B(X,Y,2,1))U  (B(X,Y,2,2)UY  = B(X,Y,2,4)

X =  2., MIXED = (B(X,Y,3,1))U  (B(X,Y,3,3))UX = B(X,Y,3,4)

Y =  3., MIXED = (B(X,Y,4,1))U  (B(X,Y,4,3))UY = B(X,Y,4,4)
```

26, line 3, "valid" misspelled

26, last 4 lines, delete

34, 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

```
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 CDS6500, 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

2DEPEP: The name has been changed to P2C0-TRIANGLES. This is not the same software as sold by IMSL with the name 2DEPEP.

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 P3C1 COLLORDER.

YALE ENVELOPE: See YALE SPARSE note.

<u>NESTED DISSECTION</u>: This indexing is now available for three dimensional problems. The possible values for the parameter are:

NDTYPE = 5	5 point nested dissection (2 DIM)
NDTYPE = 9	9 point nested dissection (2 DIM)
NDTYPE = 7	7 point nested dissection (3 DIM)
NDTYPE = 27	27 point nested dissection (3 DIM)

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.

Discretization		Indexing		Solution	
1.	5-POINT STAR	14.	NATURAL	20.	LINPACK BAND
2.	7-POINT 3D	15.	RED-BLACK	21.	LINPACK SPD BAND
3.	PC-C1 COLLOCATION	16.	YALE MIN DEG	22.	SPARSE GE-PIVOTING
4.	P3-C1 GALERKIN	17.	YALE RCM	33.	SOR
5.	HODIE-HELMHOLTZ	32.	NESTED DISSECTION	34.	JACOBI SI
6.	HODIE-ACF			35.	JACOBI CG
8.	HODIE 27-POINT 3D	41.	P3C1 COLLORDER	36.	SYMMETRIC SOR SI
9.	FFT 9-POINT			37.	SYMMETRIC SOR CG
10.	P2C0 TRIANGLES			38.	REDUCED SYSTEM SI
11.	MARCHING ALGORITHM			39.	REDUCED SYSTEM CG
12.	DYAKANOV-CG			30.	YALE SPARSE
13.	DYAKANOV-CG			31.	YALE ENVELOPE
40.	FISHPAK HELMHOLTZ				
42.	YALE GALERKIN				

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.

MODULE	MAY BE FOLLOWED BY
1	14, 15, 16, 17, 32
2	14, 15, 16, 17, 32
3	14, 41
4	14, 16, 17, 32
5	14, 16, 17, 32
6	14, 16, 17, 32
8-13, 40	None
14	20, 21, 22, 30, 31, 33, 34, 35, 36, 37
15	30, 31, 38, 39
16	22, 30, 31
17	22, 30, 31
32	22, 30, 31
41	20, 33, 34, 35, 36, 37
42	14, 16, 17

Figure A4. Module Compatibiliy 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 4×4

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 solution 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, otherwise a solution is obtained to an essentially different problem. This comparison should always be made to insure that a meaningful solution has been obtained. The value of PERTRB is printed if LEVEL$\geq$2.

Fishpak will attempt to find a solution even if $\lambda>0$ in which case a solution 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*NGRIDY + (13 + INT(LOG_2(NGRIDX)) *NGRIDX. The Execution time is roughly proportional to NGRIDX*NGRIDY*LOG_2(NGRIDY), but also depends on the boundary conditions.

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 4×4 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 4×4 block.

See Dyksen, W. R., "A New Ordering Scheme for the Hermite Bicubic Collocation Equations", Purdue University, Computer Science Department Report CSD-TR 364, May 1, 1981.

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.

<u>MODULE NAME</u>: P2C0 TRIANGLES *

<u>AUTHOR/DATE</u>: G. Sewell, 10/16/78

<u>INITIAL/FINAL INTERFACE</u>: EQUATION FORMATION-OUTPUT

<u>RESTRICTIONS</u>: Two-dimensions, self-adjoint

<u>MODULE DESCRIPTION</u>: 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.

<u>PARAMETERS</u>: 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.)

<u>FORTRAN</u>: 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_j,Y_j)*H_j**3 uniformly, where (X_j,Y_j) is the center of triangle j and H_j is its diameter. If D3EST is an estimate of the function

$$\max_{i+j=3} \left| D_x^i D_y^j u \right|$$

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

* This was formerly named 2DEPEP, it is not the software sold by IMSL under that name.

ELLPACK LITERATURE

1976 Rice, John R., ELLPACK - A Cooperative Effort for the Study of Numerical Methods for Elliptic Partial Differential Equations, CSD-TR 203, October 15, 1976 (5 Pages).

Rice, John R., ELLPACK Contributor's Guide, CSD-TR 208, November 1, 1976 (Revised September 16, 1977) (45 Pages). Obsolete.

1977 Rice, John R., ELLPACK: A Research Tool for Elliptic Partial Differential Equations Software, in Mathematical Software III, (J. Rice, ed.), Academic Press, 1977, pp. 319-341.

Rice, John R., ELLPACK: A Cooperative Effort for the Study of Numerical Methods for Elliptic Partial Differential Equations, in ARO Report 77-3: Proceedings of the 1977 Army Numerical Analysis and Computer Conference, pp. 165-169.

Rice, John R., ELLPACK 77 User's Guide, CSD-TR 226, March 18, 1977 (Revised January 20, 1978, Corrected March 27, 1978) (34 Pages). Replaced by CSD-TR 289 September 15, 1978 (69 Pages) with the same title. Revised July 1, 1980.

Houstis, Elias N. and Rice, John R., Software for Linear Elliptic Problems on General Two Dimensional Domains, in Advances in Computer Methods for Partial Differential Equations II (R. Vishnevetsky, ed.), IMACS, New Brunswick, NJ (1977), pp. 7-12.

Boisvert, Ronald F., ELLPACK Distribution Guide, CSD-TR 254 December 7, 1977 (Revised September 15, 1978). (21 Pages).

1978 Lynch, Robert E. and Rice, John R., The HODIE method and its performance, in Recent Advances in Numerical Analysis (C. de Boor, ed.) Academic Press, 1978, pp. 143-175.

Houstis, Elias N. and Rice, John R., A Population of Partial Differential Equations for Evaluating Methods, CSD-TR 263, May 15, 1978 (76 Pages). (Replaced by MRC reports, April, 1980)

Houstis, Elias N. and Rice, John R., An Experimental Design for the Computational Evaluation of Elliptic Partial Differential Equations Solvers, CSD-TR 264, May 1978 (17 Pages).

Rice, John R., ELLPACK 77 Contributor's Guide, CSD-TR 267, June 10, 1978 (34 Pages).

Gherson, P., Lykoudis, P. S. and Lynch, R. E., The Use of ELLPACK 77 for Solving the Laplace Equation on a Region with Interior Slits, Application to a Problem in Magnetohydrodynamics, CSD-TR 275, July 1978.

Boisvert, R. F., Houstis, E. N. and Rice, J. R., A System for Performance Evaluation of Partial Differential Equations Software, CSD-TR 278, July 28, 1978 (22 Pages). IEEE Trans. Software Engineering, 5 (1979) pp. 418-425.

Rice, John R., ELLPACK Workshop, CSD-TR 285, August 1978 (14 Pages).

Boisvert, Ronald F., and Bonnet, Jay M., The Data Management Subsystem of the System for Performance Evaluation of PDE Software, CSD-TR 286, August 30, 1978 (22 Pages).

1979 Rice, John R., Programming Effort Analysis of the ELLPACK Language, CSD-TR 288 (3 Pages). SIGNUM Newsletter, 14 (1979) pp. 109-111.

Rice, John R., ELLPACK 78 User's Guide - Preliminary version, CSD-TR 306, May 9, 1979.

Rice, John R., and Sewell, Granville, On the effectiveness of iteration for the Galerkin method equations, CSD-TR 307, June 1, 1979.

Boisvert, R. F., Rice, J. R., and Warner, J., ELLPACK network documentation - preliminary version, CSD-TR 308, July 15, 1979.

Boisvert, R. F., ELLPACK Control Card Procedures: XEQ ELLPACK, XEQ GETELL, CSD-TR 310, August 27, 1979 (15 Pages).

Rice, J. R., 1979 ELLPACK Workshop, Progress report and proposal for a 2-year program, CSD-TR 315, August 15, 1979 (Revised, November 15, 1979) (16 Pages).

Boisvert, R., Brophy, J., Rice J. and Warner, J., ELLPACK Network Users Guide, CSD-TR 319, December 1979 (35 Pages).

1980 Rice, John R., Houstis, E. N. and Dyksen, Wayne, A Population of Linear, Second Order, Elliptic Partial Differential Equations on Rectangular Domains, Part 1 and 2., Mathematics Research Center Technical Reports 2078, 2079. Math Comp. 36, (1981) pp.

Boisvert, R., Recommendation for ELLPACK module standards, NBS Scientific Computing Division Report, March 26, 1980 (14 Pages).

Houstis, E. N. and Rice, J. R., An Experimental Design for the Computational Evaluation of Elliptic Partial Differential Equation Solvers, in Production and Assessment of Numerical Software (M. Hennell and L. Delves, eds.) Academic Press pp. 55-65.

Houstis, E. N. and Rice, J. R., High Order Methods for Elliptic Partial Differential Equations with Singularities, CSD-TR 341, June 10, 1980 (26 Pages). Int. J. Numer. Meth. Engr.,

1981 Rice, J. R., Machine and Compiler Effects on the Performance of Elliptic PDE Software, CSD-TR 359, February 16, 1981.

Rice, J. R., On the Effectiveness of Iteration for the Galerkin Method Equations, in Advances in Computer Methods for Partial Differential Equations IV (R. Vishnevetsky, ed.) (1981) IMACS, New Brunswick, NJ, pp.

Rice, J. R., ELLPACK, Progress and Plans, in Elliptic Problem Solvers (M. Schultz, ed.) (1981) Academic Press, (1981) pp.

Dyksen, W. R., A New Ordering Scheme for the Hermite Bicubic Collocation Equations, CSD-TR 364, April 21, 1981 (28 Pages).

Rice, J. R., ELLPACK User's Guide Supplement, CSD-TR 363, May 1, 1981 (11 Pages).