1978

ELLPACK Workshop

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ELLPACK WORKSHOP

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ABSTRACT

This report summarizes the discussions, presentations and plans made at the ELLPACK workshop. The contents are:

1. Purpose and attendees
2. Principal topics of discussion
3. Miscellaneous items
4. Immediate plans
5. Postscript of August 1, 1978: ELLPACK status
6. Acknowledgements

Appendix A: Workshop Program

Appendix B: Discussion Topics proposed in advance of workshop.

ELLPACK WORKSHOP

1. PURPOSE AND ATTENDEES. The purpose of this workshop was to gather people together who have an active interest in the numerical solutions of elliptic PDE's in general and ELLPACK in particular in order to have a thorough discussion of the ELLPACK project. The attendees were

R. Bank	University of Texas
G. Birkhoff	Harvard University
R. Boisvert	Purdue University
P. Concus	University of California, Berkeley
W. Cowell	Argonne National Laboratory
S. Eisenstat	Yale University
A. George	University of Waterloo
R. Grimes	University of Texas
E. Houstis	University of South Carolina
D. Kincaid	University of Texas
R. Lau	Office of Naval Research
G. Leaf	Argonne National Laboratory
R. Lynch	Purdue University
J. Rice	Purdue University
D. Rose	Vanderbilt University
A. Sherman	University of Texas
M. Schultz	Yale University
W. Ward	Purdue University
D. Young	University of Texas

There were several other occassional attendess from the Argonne National Laboratory.

The workshop program is given in Appendix A and it shows the general lines of discussion well. The plan of the report is to summarize the principal topics of discussion (the ones that generate the most heat), then list a number of miscellaneous points made and to add a postscript about developments relative to these discussions that have taken place up to August 1, 1978.

2. PRINCIPAL TOPICS OF DISCUSSION. There were three topics that lead to recurring, sometimes vigorous, discussion. A brief summary is given here of the main points.

   A. The nature and techniques of software evaluation. As we would expect from a new process (software evaluation) there is not much concensus on what it is or how it should be done. Typical of the debated questions were:

      How should the error be measured? Candidates are max error, least squares error or the size of the residuals or relative value of these. Where should the error be measured? Should 100 or 200 fixed points be chosen that give no method an advantage? If so, how does one define the value of a finite difference solution off the grid? If interpolation is used, is one measuring the error of the PDE solution process or of the interpolation process? Since we have 6th order finite difference methods, how does one do 6th order interpolation of a table of finite difference values. Yet it is known that measuring the error at grid points sometimes favors some finite-element methods. If the true solution has a small region of difficulty, then measuring the error at the grid points of a coarse grid can give a totally misleading result (examples of this have already arisen).

The discussions were illuminating, but there seemed to be about as little concensus at the end as at the start.

What execution times should get charged to what modules? People attach considerable importance to the "fairness" of performance evaluation. It is inevitable that the ELLPACK framework will favor some software modules over others. An example: A discretization module generates a system of equations which are solved by a band Gauss elimination. Which module gets "charged" for the time required to rewrite the equations in the special storage format for the band matrix?

How specialized should the methods be? Is it appropriate to compare general purpose collocation with a Fast Fourier Transform method on a Poisson problem? Should all symmetric matrices always be solved by modules for symmetric matrices? The exploitation of more special properties of a problem always results in better performance. To push this to its ultimate conclusion means that each problem would have its own method. One of the design points of an evaluation is to adequately balance and account for generality versus specializations in the methods.

The design and analysis of performance evaluation experiments is still a delicate art and there are many pitfalls in avoiding bias or even its appearance.

B. The ITPACK routines. The first ITPACK routines operational in ELLPACK 77 did not smoothly fit within the framework naturally and did not interface with other modules well or at all. This had been recognized by the ITPACK group and they were redefining their data structures to achieve much more general applicability. As usual, there were 3 possible sparse matrix representations. that looked good, but none was clearly superior. The pros and cons were discussed at some length without any clearcut conclusion. No matter what was done, there would be some situations where this was not as good as one would like; this is the usual price one pays for generality. The discussions often became involved with that of indexing.

C. What should the INDEXING modules do? The original ELLPACK design included two things (at least) under indexing:

(a) reordering the equations and/or unknowns. Examples are band width minimization or nested dissection ordering.

(b) reformatting the equations or getting a new representation for the same matrix. Examples are changing a system into the band matrix storage format or one of many sparse matrix formats.

There was considerable sentiment for expanding the ELLPACK structure so as to include these separately. Reordering would be the INDEXING segment and reformatting would be a new segment. This was opposed by those that would have to make the change as it would require a substantial revision of the preprocessor.

Agreement reached:

(a) All discretization modules use the same format and representation of the linear system generated. Variable indexes would be column numbers of a matrix (even though it is not written out in full).

(b) INDEXING includes only the reordering of the linear system and not reformatting.

(c) Reformatting is to be incorporated with each solution module. If separate timing is desired (some insisted this be possible) then a simple facility is to be included to do this.

It is clear that the ultimate role of indexing and reformatting is still obscure but that it is an important part of the PDE solution process. Preliminary experience with ELLPACK 78 shows that it is even more complicated there and thus more essential to find the proper framework for handling it.

3. MISCELLANEOUS ITEMS. This section contains many points which seem to be worth recording even if they are not worth expanding upon.

A. Three Dimensional Geometry Representation. This is wide open, a general scheme is probably impossible. We should first try schemes of limited capabilities.

B. Hodie Matrix for Symmetric Problems. It is not clear that this method always, sometimes or never produces a symmetric matrix from a symmetric problem. The reasons why are not yet clear.

C. LINPACK routines should be used.

D. An EXECUTE "Name" facility should be included in SEQUENCE. No plans exist for doing this as of 8/1/78.

E. ITPACK Modules. The number and complexity of them will be reduced.

F. Consistency of DISCRETIZATION output. The current ELLPACK modules do not write the linear equations consistently.

G. The GALERKIN module should not produce a band matrix, this step should be elsewhere.

H. A 3-dimensional 7-POINT STAR module is needed badly.

I. The domain restriction on FF79 should be removed.

J. Randy Bank has a nice set of programs which can be incorporated in ELLPACK soon. They are for general separable problems.

K. The Yale Sparse Matrix Package can be incorporated into ELLPACK by fall. This is the work of Eisenstat, Gursky, Schultz and Sherman.

L. Doubt expressed that the discretization modules should use the sparse matrix representation i, j, a_{ij}.

M. There should be an array to associate variables with the geometry (grid numbers)

N. The name of the SPARSE SHERMAN module should be changed. It is now SPARSE GAUSS ELIMINATION.

O. The Purdue System for PDE/method evaluation should be made available to the other active ELLPACK sites.

P. "Dummy" modules should be included so people can experiment without changing the preprocessor.

Q. It is agreeable to let IMSL distribute ELLPACK as long as each module author has the ability to delete his programs from that version.

R. Houstis and Rice have generated a substantial population of PDE problems for ELLPACK 77: Computer Science Department, Technical Report 263, Purdue University.

S. ELLPACK 78 should have the boundary specified counterclockwise. A switch has since been introduced to allow either orientation.

4. IMMEDIATE PLANS. There was no change made in the organization and general method of operation of the ELLPACK project. The near term plans agreed upon include:

A. By the end of the summer:

(a) New ITPACK modules will be installed

(b) The preprocessor will be changed to reflect various suggestions and implications of suggestions made e.g. items M, N and P of the previous section, segmented timing for modules, SYMMETRIC switch installed

(c) Modules will be changed to correspond to the agreements on the INDEXING definition. Also some of the items C, F, G, and I should be taken care of.

(d) A new ELLPACK 77 Contributor's guide will be written with more discussion of how to add modules.

(e) A description of the Purdue PDE method evaluation system will be written and circulated.

(f) New modules will be incorporated including:

YALEPACK programs

Some of Randy Bank's programs

A 7-POINT STAR for 3-dimensions (University of Texas)

LINPACK routines

B. <u>By early fall</u>:

(a) ELLPACK 78 will become operational

(b) A new ELLPACK 77 User's Guide will be available which reflects the "final form" of ELLPACK 77 and all the modules incorporated at that time. This does not imply that further modules will not be added (they will be); it only implies that new preprocessor features are no longer contemplated.

(c) This version will be distributed to all active ELLPACK participants and, possibly, to IMSL to replace the March version they now distribute.

5. POSTSCRIPT OF AUGUST 1, 1978: ELLPACK STATUS. We indicate what has happened since the workshop and thus indirectly provide a status report on ELLPACK.

End of Summer Targets-Progress

(a) Six new ITPACK modules have been received and are being installed; all the old ones have been removed.

(b) All of the suggested preprocessor changes have been made and tested.

(c) All of the modules involved have been changed in accordance with the INDEXING agreement reached at the workshop. The required preprocessor changes have been made and tested.

(d) There is: ELLPACK 77 Contributor's Guide by J.R. Rice, CSD-TR 267, June 10, 1978 (36 pages).

(e) There is: A System for Performance Evaluation of Partial Differential Equations Software by R.F. Boisvert, E.N. Houstis and J.R. Rice, CSD-TR 278, July 28, 1978 (22 pages). A data management system has been written and tested for the experimental data; documentation is partially typed. The PDE population of Houstis and Rice has been enlarged considerably and a new version of A Population of Elliptic Partial Differential Equations in Two Variables CSD-TR 263 is about ready for typing.

(f) New modules that are ready or nearly ready for ELLPACK 77 are:

(i) two modules for the YALEPACK sparse matrix programs. One of these is parameterized to include a number of the YALEPACK programs.

(ii) two modules of Randy Bank's programs

(iii) 7-POINT STAR in 3-dimensions from the University of Texas

(iv) two LINPACK modules for Gauss elimination on hand matrices (symmetric and non-symmetric).

Early Fall Targets-Progress

(a) The extension of the ELLPACK preprocesses for non-rectangular domains is complete and somewhat tested. The ELLPACK system distributed in early fall will have many ELLPACK 78 capabilities even though the User's Guide will not mention them. The domain processor has been installed with the preprocessor and now works properly on a reasonable set of test cases. The 5-POINT STAR module for general domains is nearly operational. Some output routines are operational (e.g. PLOT-DOMAIN, TABLE-BOUNDARY) and some are not. We have the subroutines needed for the output but implementing PLOT-U or TABLE-ERROR is still likely to be tricky. It's the INDEXING problems that complicate things.

(b) The new ELLPACK User's guide has not been started.

(c) Our target date for distribution of the new ELLPACK version is late September (no promises, though).

Other Items

(a) Personnel. E.N. Houstis has left Purdue for:
Department of Mathematics and Computer Science
University of South Carolina
Columbia, SC 29208

Granville Sewell will be visiting Purdue for the 1978-79 year and he will be involved in the ELLPACK project part time.

(b) Houstis and Rice have completed a study of high order methods applied to singular problems. The results are yet to be written up but they show that high order methods are more efficient for singular problems.

(c) We will soon make a study of the effect of various compilers on the execution of the ELLPACK system and modules.

(d) Implementations of the HODIE 9-POINT STAR and P3CI-COLLOCATLUN for general domains is under way.

(e) IMSL has already sold 15 copies of ELLPACK and has a number of other orders awaiting the arrival of more copies of the User's and Distribution Guides from Purdue.

(f) The ELLPACK system is being used by some people in our engineering school. The report "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 by R.E. Lynch, P.Gherson and P.S. Lykoudis shows its use for a rather difficult Neumann problem on a rectangular domain with slits.

(g) Acknowledgements. The work of various people on the ELLPACK project is supported by individual grants and contracts. We especially thank the Office of Naval Research for providing the funds for this workshop. Gary Leaf of Argonne handled the local arrangements and we thank him and his capable assistant Pat Witkowski for making things run smoothly.

APPENDIX A

ELLPACK WORKSHOP PROGRAM

Friday, May 19

9:00 → 9:15	J.R. Rice, Opening Remarks
9:15 → 10:00	G. Birkhoff, 3-Dimensional Representations and Applications
10:00 → 10:30	Break
10:30 → 11:00	R. Boisvert, The Hodie Method for the Helmholtz Problem
11:00 → 11:45	E.N. Houstis, Evaluation of Methods for Solving PDE's
1:00 → 2:30	J.R. Rice and R. Boisvert, ELLPACK 77 Status Report
	J.R. Rice, ELLPACK 78
2:30 → 3:00	Break
3:00 → 4:30	D. Young, ITPACK: Past, Present and Future
	D. Kincaid, ITPACK User Interface
	R. Grimes, ITPACK Data Structures and Numerical Results

Saturday, May 20

9:15 → 9:35	D. Rose, Sparse Matrix and PDE Work at Vanderbilt
9:35 10:15	R. Bank, Generalized Marching Algorithm and Applications
10:15 → 10:45	Break
10:45 → 11:15	A. Sherman, The Yale Sparse Matrix Package
11:15 → 12:00	S. Eisenstat, Suggestions for ELLPACK design
1:15 → 4:30	General Discussion, J.R. Rice Moderating

A. ELLPACK 77 strengths and weaknesses

B. ELLPACK 78 strengths and weaknesses

C. Coordination of group efforts with ELLPACK at Purdue

D. Future objectives for ELLPACK

E. Future Organization, manpower, funding, etc.

APPENDIX B

DISCUSSION TOPICS PROPOSED IN ADVANCE OF THE WORKSHOP

1. Analysis of software evaluations:

   (a) How effective have iterative methods proved to be?

   (b) When should one use high order and when low order methods?

   (c) How well do finite differences do compared to finite elements?

   (d) How much more effective are special methods (e.g. Fast Fourier Transform, Tensor Products) for special problems (e.g. Poisson problem in a rectangle) than general methods applied to these same problems?

   (e) Which type of problems lead to a large payoff for sparse matrix methods, nested dissection, etc.

2. What is a good standard set of test problems to "calibrate" methods? What are the strengths and weaknesses of such calibrations?

3. Evaluation of 2-Dimensional General Geometry Representations. What are the strengths and weaknesses of the various alternatives that have been proposed?

4. Possible 3-Dimensional General Geometry Representations. Only the most straight-forward and cumbersome schemes have been tried. What are some better ways to handle 3-D geometry information.

5. Effectiveness of INDEXING Modules. These modules are designed to free the equation solvers from the particulars of operator discretization. What are the strengths and weaknesses of this approach and how can it be made more effective?

6. Use of ELLPACK as a Production Tool. What are the situations where ELLPACK is effective as a production tool (as opposed to a research tool)? How much has the research orientation of the ELLPACK group degraded the production capability of the ELLPACK system?

7. Implications for Large Systems. The experience with ELLPACK will be for small to moderate sized problems. How safely can one extrapolate these results to the large and very large problems that arise in some application areas? Which conclusions (opinions) reached in 1. above seem likely to be valid for huge applications systems?

8. Use of ELLPACK as an Educational Tool. Is it worthwhile to invest effort into ELLPACK for educational purposes? In which contexts would it be effective? How much effort is required to make it effective?

9. Future Developments. Which of the many possible avenues are going to be followed and who is going to do what? Is there real interest in developing a "production quality" version of the system and, if so, who would be interested in doing it, funding it or using it?