DRAFT VERSION: Please respond by October 1, 1979 if you have any comments, corrections or suggestions.

1979 ELLPACK WORKSHOP, PROGRESS REPORT AND A PROPOSAL FOR A 2-YEAR PROGRAM.

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ABSTRACT

The program, attendence and summary of the discussion are given for the ELLPACK Workshop held at Argonne National Laboratory, July 26-27, 1979. The discussions express the cooperative group's views on the needs, status and future hopes for the ELLPACK system. The various ideas expressed, plus others, are organized into a proposed 2-year program of work on ELLPACK. Comments and suggestions about this proposal are invited.

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1. INTRODUCTION.

The program and attendence at the ELLPACK workshop are given in the appendix. The references contain a complete list of ELLPACK references and documentation; included are several new or revised items. This workshop was supported by the Department of Energy and thanks is due to Paul Messina and Doris Pahis for making the local arrangements.

2. PROGRESS REPORT.

The highlights of the progress since the summer of 1978 are given below. New technical articles and reports can be found in the references.

A. ELLPACK 78. The general geometry facility in 2-dimensions was put into ELLPACK along with two discretization modules to use it. Several of the solution modules can be used unchanged with these modules. The ELLPACK 78 system is actually contained in the ELLPACK 77 system version of April 1977 being distributed by IMSL. A contour plotter for general geometry was developed.

B. ITPACK 2.0 The more flexible and efficient implementations of the iterative methods have been made and they were incorporated into the ELLPACK system version of August, 1979.

C. ELLPACK NETWORK. A network facility for access to ELLPACK has been started. As of August 1979 members of the cooperative group can telephone the Purdue computer and run ELLPACK programs using special user oriented commands. One can also access the data base of performance statistics through the network.

D. MODULES. In addition to a complete set of new ITPACK modules, the following modules were also put into ELLPACK:

a. YALE RCM (Aug, 1979): Part of YSMP(YALE SPARSE MATRIX PACKAGE); an indexing module

b. YALE ENVELOPE (Aug, 1979): Part of YSMP; sparse matrix solvers

c. 2DEPEP (March, 1979): A self contained finite element code with triangular mesh refinement.

d. FFT9(IORDER = 2) (Aug, 1979): A second order version of FFT9.

e. OTHERS. The following were added to ELLPACK in the summer or fall of 1978.

HODIE-HELMHOLTZ	MARCHING ALGORITHM
DYAKANOV-CG	DYAKANOV-CG4
YALE MIN DEG	YALE SPARSE
LINPACK BAND	LINPACK SPD BAND

In addition, versions of 5-POINT STAR and 2DEPEP have been included which handle general geometry.

E. TESTING/EVALUATION. Substantial progress was made on various efforts related the evaluation of PDE software. The efforts are:

a. PDE POPULATION: A set of 184 PDE's for ELLPACK 77 been created and tested out, a writeup is in progress.

A population of PDEs and parameterized domains for ELLPACK 78 has been developed.

b. SINGULARITIES STUDY: A broad study of the effect of singularities and other troubles was almost completed (data for FFT9(IORDER = 2) still needs inclusion in the study)

c. ITERATION FOR GALERKIN EQUATIONS: A small study suggests that the relationship between iterative and direct methods for the linear system from Galerkin discretizations is the same as for 5-point star discretizations

F. FACILITIES. Programs were completed for standard analysis and plotting of data from the performance evaluation data base.

3. DISCUSSION SUMMARY.

There were two discussion sessions, one for "technical" issues and one for "organizational" issues. A list of topics was distributed beforehand (see the program in the appendix) and most of these topics were covered at some point during these two sessions. We summarize the remarks and ideas which seems to be the most interesting.

A. NEW FACILITIES. Considerable interest was expressed in extensions of ELLPACK such as nonlinear equations, time dependent problems, adaptive mesh refinements, etc. While some of these are currently possible within ELLPACK, an elegant implementation would require some substantial new facilities and interfaces. No consensus was reached on what should be done or how much effort it would be.

B. MODULE STANDARDS. The standards need more precision. A lengthy discussion took place over the fact that GALERKIN followed by YALE SPARSE does not work. The reason is that GALERKIN produces

a symmetric matrix in a symmetric form (only half the matrix is stored) while YALE SPARSE expects a symmetric matrix to be given in full. It is not obvious who should have the responsibility of copying in the second half from the symmetric form, through the contributors guide says it's the discretization module. The coordinator suggested that Galerkin not waste this space as several solution modules do not need the second half.

Almost every module violates one or more of the following requirements:

a) AUTHORS NAME: prominently displayed in program

b) USER DOCUMENTATION: A page giving adequate information and references for use and understanding.

c) COMMENTS: Good internal documentation

d) PORTABILITY: Standard Fortran coding used.

e) OUTPUT: Meaningful messages under control of user.

f) FAILURE ACTIONS: Standard messages and setting of switch when an impossible situation is met.

It was agreed that some mechanism is needed to clarify and enforce module standards. Purdue does not have the manpower or inclination to make non-trivial modifications to modules.

Sentiment was expressed that the ELLPACK system should take more responsibility for checking compatibility at module interfaces. This was originally planned, but was found highly non-trivial to implement. The table in the User's guide is complicated to use.

C. <u>EASE OF USE.</u> Suggestions for improving ELLPACK for the user were:

1. Labelling the timing output with the name of the module.
2. More freedom of expression in defining domains
3. A breakdown of the memory used by modules.

D. SYMMETRY. The opinion was expressed that a symmetric matrix should be generated from a self-adjoint operator. The modules do not always do this on general domains and it is not clear how to guarantee this.

E. NETWORK. Suggestions for improving the network were made and the plans for the new version to be released shortly were outlined. The new version will allow group members to make new data runs and have the results entered into the data base.

F. PDE SOFTWARE EVALUATION. The data base needs to be able to accomodate evaluation data from other computers, there needs to be a way to enter data from sources outside Purdue. It would be nice if other group members can run for themselves the PDE population(easy to do), the ELLPACK program synthesis system (not hard to do) and the data base system (this would require a new data base system, hence is hard to do). Care must be taken when codes are significantly changed then the corresponding new data is separately identified.

A important shortcoming of the present data set is that the Purdue computer has a small memory which severely limits problem size.

G. ELLPACK VARIANTS. ELLPACK can be used by the network or, by getting a copy or by getting and modifying a copy. The pros and cons of allowing group members to modify their copies of

ELLPACK were discussed at length. People who want to expand ELLPACK's facilities or use need to change it; others want to know that ELLPACK is stable over time. The most widely supported suggestion was to have a "core" ELLPACK 78 upon which extensions and variants could be based.

H. EDUCATIONAL USE. Several people have used ELLPACK in their courses and the students found it easy to use. Interest was expressed in making ELLPACK even more suitable for classroom use. A voluntary committee was formed to explore this further (Sherman = Chairman, Birkhoff = Secretary, Young).

I. FUTURE DEVELOPMENT. The consensus was for keeping to ELLPACK's original goal as a software development and evaluation tool. As ELLPACK matures it will probably receive substantial educational and applications use, but no enthusiasm was expressed for developing a production oriented system. Additional capabilities were discussed at length and with much interest, but no decision reached on which were the most desireable or likely. More finite element type modules are needed.

The hope was expressed that at some future time ELLPACK (or a version of it) would become a stable system and that its distribution and routine maintenance could be taken over by some appropriate organization.

J. MANAGEMENT AND FUNDING. The current management (Rice as coordinator at Purdue) will be continued. Each person will arrange his own funding to work on ELLPACK or related efforts. It was proposed that the ELLPACK group have a secretary (at Texas?) who would be a central source for communicating news, etc.

It was proposed and agreed that the next ELLPACK workshop be held in New Haven with the Yale group as hosts.

4. OUTLINE OF PROPOSED 2-YEAR PLAN.

The ideas presented at the workshop have been meshed with others to generate a proposed plan for the next 2 years of work on ELLPACK. This plan is presented here in outline form and then expanded upon in later sections:

I. CORE ELLPACK 78.

A. Basic concept is current design, Improve various things and enforce module standards.

B. New facilities: HOLE and 3-dimensional cylinders.

C. More terminal and network oriented output

D. Additional modules: We hope for

Rectangular: HODIE ACDEF, more finite element type, FFT in 3 dimensions

General : HODIE, P3C1-COLLOCATION, 7-POINT STAR on cylinders.

Other modules will be welcomed.

E. More complete documentation for users, contributors, system installation and data base access.

II. PREPROCESSOR REWRITE

A. Complete rewrite is part of another effort (TOOLPACK)

B. Should make it substantially easier to maintain, modify or extend ELLPACK.

III. EDUCATIONAL USE

A. Allow for inclusion of "non-competitive" modules like general Gauss elimination, Gauss-Seidel iteration, O(h) discretizations, etc.

B. Student oriented user's guide.

IV. SOFTWARE EVALUATION SYSTEM

A. Use for a variety of studies

B. Extend data base system to allow for data from different computers. Provide mechanism for accepting data from group members and (roughly) comparing results from different machines.

V. EXTENSIONS

A. Initiate design analysis, make the new preprocessor amenable to the expected extensions

B. Extensions to be considered first:

Automatic coordinate transformations

A "stepping" interface (nonlinear or time dependent problems)

VI. IMPLEMENTATIONS AT PURDUE

(1) VAX (under UNIX operating system) with 2½ million bytes of core; also virtual memory.

(2) CDC 6600 (which is trivial to do)

5. CORE ELLPACK 78

No attempt is made to describe "core" ELLPACK 78 here as that would repeat material already available in other places. The enforcement of module standards will start with a better statement of the standards, followed by a report to module authors on the shortcomings of their modules. It is expected that they will then make the changes required.

Some additional modules are listed in the outline, but recall that the original design of ELLPACK is open ended on the number of modules. Thus even core ELLPACK 78 is not expected to be static in this regard, modules of interest to PDE software evaluation are expected to be added indefinitely.

The documentation of core ELLPACK 78 is expected to be substantially improved. Module contributors will be required to prepare more complete descriptions with references to the literature for further information. An average length of 2 pages seems appropriate.

6. PREPROCESSOR REWRITE

One aspect of the TOOLPACK effort is to prepare portable programs that facilitate writing Fortran preprocessors. It is hoped that work on TOOLPACK will start in 1980 and that the preprocessor facilities will be among the first to be done. The plan for TOOLPACK includes a complete rewrite of the ELLPACK preprocessor to evaluate and test the preprocessor facilities.

It is hoped that these facilities will make preprocessor production easier and the resulting software more transparent and maintainable. This will be an obvious time to incorporate improvements into ELLPACK and to make changes that accommodate future extensions of ELLPACK 78.

7. EDUCATIONAL USE

The committee on educational use of ELLPACK will survey the needs in this direction. One can conjecture, for example, that modules will be suggested which are for educational use only. The core ELLPACK 78 will accommodate itself to educational use and group members are encouraged to try it in the classroom.

8. SOFTWARE EVALUATION SYSTEM

ELLPACK and the associated system for the evaluation of PDE software are ready for use in evaluation studies. Several will

be made in the next two years.

Two extensions of the PDE software evaluation system are planned: (a) inclusion of data from different machines,(b) a technique for rough conversion of data for one machine to another. This will allow the data base to accept data from outside Purdue, though, naturally, contributors must be of a substantial nature before a new machine data is accepted. Additions to the data base (for machines already accommodated) by group members away from Purdue will be facilitated.

9. EXTENSIONS

Several extensions of ELLPACK have been proposed and the first step of an extension is to make a fairly precise analysis of how the extensions should be done and what types of PDE software and problems would be involved. It is expected that at least two extensions will be analyzed in detail in the next year: automatic coordinate transformations and mildly nonlinear elliptic problems.

10. IMPLEMENTATIONS AT PURDUE

The ELLPACK system at Purdue is in the process of being moved to the VAX under the UNIX operating system. This will give a machine with large core (2½ megabytes = 625,000 words of 7 decimal digits or 312,000 words of 15 digits) and virtual memory (not yet supported by UNIX). The Purdue computing center just added a CDC 6600 and the ELLPACK system will run on it without any change or transfer of software.

ELLPACK WORKSHOP PROGRAM

*** FINAL VERSION ***

THURSDAY, JULY 26		
9:00 - 10:30	General Description of ELLPACK:	J. Rice
	Personnel	R. Boisvert
	ELLPACK 77 and ELLPACK 78	
	Performance Evaluation System	
10:30 - 11:00	Break	
11:00 - 11:40	ELLPACK Network	R. Boisvert
	Lunch	
1:15 - 3:15	The ITPACK Project	D. Kincaid
	Current Status	D. Young
	Comparison Studies	
	Future Plans	
3:15 - 3:45	Break	
3:45 - 4:30	Network Demonstration	R. Boisvert
FRIDAY, July 27		
9:00 - 9:30	Comparisons of packages for large, sparse systems	A. Sherman
9:30 - 10:00	Comparisons of finite element methods	A. Weise
10:00 - 10:30	Break	
10:30 - 12:15	Analysis of the ELLPACK System	
	General Discussion (See Attached Sheet)	
	Lunch	
1:30 - 3:30	Organization of the ELLPACK Project	
	General Discussion (See Attached Sheet)	

SESSION C: ANALYSIS OF THE ELLPACK SYSTEM

Technical topics for discussions

1. Analysis of software evaluations:
   (a) When are iterative methods preferable to good direct methods for linear problems?
   (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 an mxm 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. The PDE population of Houstis and Rice to "calibrate" methods? What are its strengths and weaknesses?
3. Evaluation of the 2-Dimensional General Geometry Representation. What are the strengths and weaknesses of the alternative that has been implemented?
4. Possible 3-Dimensional General Geometry Representations.
   Only the most straight-forward and cumbersome schemes have been investigated. What are some better ways to handle 3-D geometry information.
5. Effectiveness of the new INDEXING Modules. These modules are designed to free the equation solvers from the particulars of operator discretization. What are the strengths and weaknesses of the approach agreed upon at the last workshop.
6. Use of ELLPACK as an Educational Tool. How effective is ELLPACK for educational purposes? In which contexts is it most effective? How much effort is required to make it more useful?
7. Use of ELLPACK as a Production Tool. How effective is ELLPACK as a production tool as opposed to a research tool? How has the research orientation of the ELLPACK group affected the production capability of the ELLPACK system?
8. Implications for Large Systems. The experience with ELLPACK will be primarily for small to moderate sized problems. (that is, 20 to 500 unknowns) 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?
9. ELLPACK Network. How feasible is it to form a telephone network for the group to use the system at Purdue? What technical and user interface problems are foreseen? Is it worth the effort?
10. Future Developments. Should essentially new capabilities be added (e.g. systems of PDEs, nonlinear PDEs) in addition to adding modules to the present system? What are the technical problems associated with the new capabilities?
11. System for PDE Software Performance Evaluation. How effective is this system? Can it be used successfully by people outside Purdue? How convincing are the statistical studies that have been made using it?

SESSION D: ORGANIZATION OF THE ELLPACK PROJECT

Topics for Discussion of the ELLPACK Project.

I. Future Development Alternatives (B is the current goal)

(A) Wither away
(B) Moderate increase in modules, use for software evaluation
(C) Substantial production use by
    1. Direct application
    2. Use of modules/control program as a basis for software development.
    3. Educational applications.
(D) Significant Additions to Capabilities:
    1. Automatic Coordinate Transformations
    2. Non-linear elliptic problems
    3. Simultaneous equations
    4. Time dependent problems
    5. General 3-D geometry
(E) New, production oriented system, actively promoted as a
    1. Non-profit, essentially free system
    2. Non-profit, but self supporting system
    3. Commercial product

II. Management and Funding

(A) Adequacy of current organization/funding for current goals.
    1. Management at Purdue
    2. Personnel Costs: Faculty, Assistants, Support (Clerical or Programming)
    3. Computer costs
(B) Impact of Future Growth Alternatives
    1. Many more modules: effect on management, funding, documentation.
    2. Educational use: effect on management, funding, documentation.
    3. Production use: effect on management, funding, documentation.
    4. New Systen: effect on management, funding, documentation.
    5. New Capabilities: effect on management, funding, documentation.

III. Use of ELLPACK Software

(A) For studies of performance. Is use automatically granted?
(B) For use of others via
    1. Purdue's system, on-campus users
    2. Purdue's system, network arrangement
    3. Purdue distribution to other group members
    4. IMSL distributions
    5. Secondary distributions
    6. A new system which is self supporting or profit-oriented

IV. Role of Contributors:

(A) Maintenance, Fixing Errors Responsibilities
(B) Portability, Documentation Responsibilities
(C) How open should we be to contributors
    Impact on the size of system
    Impact on the quality
(D) Should certain software be solicited? If so, where?

ELLPACK WORKSHOP ATTENDEES

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