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ELLPACK--A Cooperative Effort for the Study of Numerical Methods for Elliptic Partial Differential Equations

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ELLPACK

A COOPERATIVE EFFORT FOR THE STUDY OF NUMERICAL METHODS FOR ELLIPTIC PARTIAL DIFFERENTIAL EQUATIONS

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ABSTRACT

This report outlines the history, the long term and short term objectives and the technical operation of the ELLPACK group. This cooperative group was formed in September, 1976 with John R. Rice as coordinator. The objective is to develope a research and educational tool for the study and evaluation of numerical methods for solving elliptic equations in 2 or 3 dimensions. It is plausible that this tool might someday form the basis for user oriented, production software for these equations. Two versions, ELLPACK 77 and ELLPACK 78, have been started to test the feasibility of this approach. The framework for ELLPACK will be developed at Purdue and technical information for contributors and research users will be provided by other reports.

ELLPACK

John R. Rice

1. HISTORY AND CURRENT ORGANIZATION. The initial impetus for a cooperative effort came from G. Birkhoff who wanted to set up formal cooperation between himself and groups at Purdue and the University of Texas. Birkhoff has a long term interest in elliptic equations and wanted to systematically test some ideas and eventually produce a modest, but useful, integrated set of programs for elliptic equations. At Purdue, E. Houstis, R.E. Lynch and J.R. Rice have been engaged in the systematic evaluation of certain methods for elliptic equations and this involved writing a coordinated set of programs embodying different methods. At Texas, D. Kincaid and D. Young have been studying iterative methods for linear systems of equations and these are particularly applicable to certain elliptic problems. They have initiated a set of programs called ITPACK which make these methods easily used.

Discussions started in the summer of 1975 about cooperating in this area and for the next year this idea was developed and crystalized. In the summer of 1976 James Ortega of ICASE felt that a broader group might be interested in this and he organized a small meeting to explore the various viewpoints. Those in attendance were

G. Birkhoff	Harvard Univ.
A. Brandt	Weizman Institute
G. Fix	Carnegie-Mellon Univ.
A. George	Univ. of Waterloo
G. Golub	Stanford Univ.
J. Ortega	ICASE
J. Rice	Purdue Univ.
M. Schultz	Yale Univ.
R. Sweet	Nat. Cent. Atmospheric Res. and Univ. of Denver
R. Varga	Kent State Univ.
O. Widlund	New York Univ.
D. Young	Univ. of Texas

Two days of discussion led to the conclusion that there was mutual interest in a cooperative effort and a framework was outlined which seemed to accommodate a number of people's work and interests. The two short term projects discussed later were agreed upon as the place to start and John Rice was selected as coordinator and benevolent dictator for the ELLPACK effort.

The ELLPACK organization is completely voluntary. Purdue will provide the software framework and define the various interfaces precisely. Contributors can prepare programs which fit into this framework and Purdue will incorporate them into ELLPACK. It is assumed that contributors will submit quality, highly portable programs to ease the burden of integrating programs into ELLPACK.

2. LONG TERM OBJECTIVES. The primary objective of ELLPACK is to be a tool for research in the evaluation and development of numerical methods for solving elliptic partial differential equations. Various components can be interchanged and the resulting accuracies, efficiencies, etc. can be measured. A person interested in one aspect of the problem (e.g. operator approximation, linear equation solution, geometric difficulties) can use other people's software for those aspects where he has less interest and expertise.

ELLPACK's use as a research tool will depend to a considerable extent on the convenience, flexibility and modularity of its framework. Thus it will be suitable for educational use in the classroom. Students will be able to see how various methods perform on various kinds of problems. Similarly, ELLPACK is expected to be of considerable use to other users who have easy or moderately difficult problems. It is not intended that ELLPACK be directly applicable to the very complex problems that arise in many areas (e.g. temperature distribution in a nuclear power plant or in a rentry

vehicle). Nevertheless, the ability to quickly solve a variety of reasonable problems should be valuable in many areas.

It is plausible to expect that if ELLPACK is successful then it will be used as the basis for user oriented, production quality software. That is, someone can examine the capabilities of the various components, select those that he feels are most appropriate and build a software system from them which is more reliable, can handle larger problems and is more efficient. This eventuality is some years in the future.

3. SHORT TERM OBJECTIVES. The first project is ELLPACK 77 where many of the programs will merely be adaptations of existing programs. Even so, it will be a complete package with a reasonable user interface and capable of solving a range of interesting problems. One of its primary objectives is to test the concept of a modular approach using interchangeable software parts.

ELLPACK 77 is restricted to rectangular geometry in 2 or 3 dimensions. Anticipated capabilities include:

Operator Approximation

2-Dim: 5-point star, 9-point star, Collocation and Galerkin with Hermite cubics

3-Dim: 7 point star, 27-point star

Special Options: Poisson Problem, Constant Coefficients, Self Adjoint Form.

Equation Solution

Direct Elimination (Band or Profile)

Nested Dissection

"Fast" Methods

SOR, Accelerated Jacobi, etc.

Conjugate Gradient

The ELLPACK group will probably meet in the Fall of 1977 to assess the prospects of ELLPACK based on the progress with ELLPACK 77.

The second project is ELLPACK 78 which is hoped to contain most of the capabilities of ELLPACK, at least in some form. The primary extension is to non-rectangular geometry, an area where some group members are already active. Other directions to be following include

a. Standard automatic changes of variables

b. Enhancement of rectangular domain capabilities

c. More operator approximations, e.g.

HODIE methods, Hermite cubics in 3 dimensions,

Method of particular solutions

d. More equation solvers, e.g.

Cyclic Chebyshev, Automated selection of SOR parameters

e. Parallel processor implementation

f. More combinations of components allowed

It is hoped that a significant part of these capabilities will be implemented by late 1978. At that point the ELLPACK effort will be evaluated and future efforts, if any, laid out.

4. TECHNICAL OPERATION. The framework and ELLPACK specifications will be specified by the Purdue group. Careful attention will be given to making ELLPACK compatible with a wide range of interests and to making it "easy" to contribute to ELLPACK. On the other hand, success depends on certain uniform standards and conventions and there is no doubt that choices will be made that some contributors find inconvenient.

It is assumed that contributors are experienced in producing portable, understandable and quality software. Purdue does not have the resources to massage poor software for incorporation into ELLPACK. The main technical

document is the Contributor's Guide to ELLPACK which is to precisely define the ELLPACK environment for a potential contributor. There will also be a shorter User's Guide and a guide to implementing ELLPACK at locations other than Purdue. Draft versions of the contributor's guide will be available in the fall of 1976 and this document will no doubt evolve considerably through the ELLPACK 77 development.