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Potential Evaluation Directions for ELLPACK

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Abstract

This report considers the potential directions of evolution of ELLPACK into a more general PDE solving system. The status and background is summarized (mostly by reference to other reports) and the options presented. The context of existing projects is outlined and the possible goals for future work presented. Conclusions are not drawn as this is the background paper for a workshop to critically evaluate the evolution of ELLPACK.

1. INTRODUCTION

The purpose of this report is to provide a framework and the background for critically evaluating the directions for the future evolution of ELLPACK. We use the name ELLPACK for future systems so as not to bias the selection of new names, it is unlikely that ELLPACK will be appropriate indefinitely.

The next two sections describe the status and background material for ELLPACK. This is accomplished primarily by pointing to papers and reports that should be available while considering this report. The fourth section then presents the directions under the broad categories of A) broader scope (or application area), B) parallel and/or distributed versions, C) increased algorithmic power, and D) user interface. This is done with five figures in a tree-like format. The next two sections briefly outline the ongoing related projects and present the goals and anticipated resources available for the project. From these are derived priorities for the general directions of evolution.

Even in the highest priority directions we cannot do all the things envisaged. The next step is to create a plan that does enough to meet the goals and which is reasonably possible within the limits of the available resources.

For completeness, the appendix gives an updated listing of the ELLPACK literature since the inception of the project.

2. ELLPACK STATUS

There are three ELLPACK systems in existence. The basic one is the batch processing version (which we just call *ELLPACK*) that has been widely distributed for several years. It is a stable, well defined and rather reliable software system.

The second system is *Interactive ELLPACK* which has existed for some time and is undergoing its third re-implementation. It is expected to be complete this summer and to become a stable, widely distributed system. It will be less portable than ELLPACK and "guaranteed" to work only on a SUN workstation with X-windows and color graphics. It should be easily ported to some other workstation with closely related software (e.g., Berkeley UNIX, X-windows, compatible graphics). This system has been started by Wayne Dyksen and Calvin Ribbens with John Bonomo now helping with the final version.

The third system is *Multiple Domain ELLPACK* which is a version of Interactive ELLPACK. It contains a variety of facilities to support domain mapping techniques for solving PDEs and it automatically creates multiple domains as the problem is transformed. This system is robust enough to be usable by others, but it must be considered an experimental prototype. Some of the basic algorithms used here are still in the early stages of maturity.

3. BACKGROUND INFORMATION

We briefly describe the contents of several papers or reports that provide background for this report. We assume that the reader is generally familiar with much of their contents.

A. *ELLPACK Project Status Report* by Rice, Dyksen, Houstis and Ribbens, CSD-TR-579, March 17, 1986, 31 pages.

Section III of this report is New Directions and has 17 pages of discussions and examples.

B. *ELLPACK: An Evolving Problem Solving Environment* by Rice, in Problem Solving Environments for Scientific Computing (B. Ford and F. Chatelin, eds) Elsevier North-Holland (1987), pp. 233-241.

This is another discussion of the topic of this report.

C. *Interactive ELLPACK* by Dyksen and Ribbens, ACM Trans. Math. Software, **13** (1987), pp. 113-132.

This is a technical description of the Interactive ELLPACK system.

D. *Computing About Physical Objects* by Bajaj, Hoffmann, Houstis, Korb and Rice, CSD-TR-696, 63 pages.

This is an overview of a large project that has an "evolved" ELLPACK as a large component. This report describes the overall objectives for a 5 year project, the specific plans are still being formulated.

E. *Supercomputing About Physical Objects* by Rice, in *Supercomputing* (Houstis, Papatheodorou and Polychronopolous, eds.), Lecture Notes in Computer Science 279, Springer-Verlag (1988), pp. 443-455.

This discusses in more detail the goals and approaches of the above project in the area of solving PDEs. The emphasis is on parallel and distributed computing.

F. *A Computational Framework for Constructing Adaptive Grid Domain Mappings* by Ribbens, CSD-TR-673, April (1987), 14 pages.

This report describes the basis of the Multiple Domain ELLPACK. There is no independent description of it. More information is contained in Ribbens' 1986 Ph.D. thesis: Domain Mappings: A Tool for the Development of Vector Algorithms for Numerical Solutions of Partial Differential Equations.

G. *Geometric Domain Processing* by Bajaj, Cui and Rice, Preliminary Draft, March, 1988.

This report outlines the current project to develop new 2D and 3D domain processors. The 2D output would be compatible with the current ELLPACK system, but the approach is changed so that the 2D and 3D algorithms are naturally related.

For completeness, the appendix of this report contains an updated list of the ELLPACK literature.

4. DIRECTIONS FOR EVOLUTION

ELLPACK might evolve in the four main directions presented in Figure 1. More detail is given in Figures 2A, 2B, 2C and 2D. Only brief remarks are given here to define these directions. We assume the reader is familiar with the documents which discuss many of these directions. Further, there is an enormous number of combinations of directions. Some directions are almost "orthogonal" to one another, e.g., adding a multigrid method, accessing MACSYMA and implementing domain mappings interact very little. Other combinations are tightly coupled, e.g., adding time dependence, general 3D shapes, access to a CAD system and an expert problem solver results in much more work than the sum of the four additions separately.

Space limitations preclude complete definitions of all these directions even though some of them are vaguely defined. The direction with the most uncertainty of definition are

Multiple ELLPACKs
Distributeed Problem Solving
Software Integration with a CAD, Structures or other PDE System
Specialization of front ends

5. CONTEXT OF ONGOING PROJECTS AND RESOURCES

We describe projects at Purdue which are related in some direct way to ELLPACK or an evolution of it. These projects define in many ways the practical and currently intended directions of evolution.

A. *Computer About Physical Objects* (CAPO). This project has ambitious goals to develop a prototype system for general simulation of physical objects. The 5 year budget is about $5 million and provides good equipment, considerable support staff (5-8 grad students, 0-2 post docs, 2-4 programmers). Several of the efforts are direct evolutions of ELLPACK (the Mathematical Software component of the project). A definitive plan for this project is still to be formulated.

B. *Interactive ELLPACK.* This project is to produce the "final" version of Interactive ELLPACK. Its target date is summer 1988. The work by Dyksen and Bonomo is supported in part by CAPO.

C. *Expert ELLPACK.* This project is to develop an expert system front end for ELLPACK. Considerable progress has been made and a draft exists of the report Elliptic Expert: The Design of an Expert System for Partial Differential Equations by Wayne Dyksen and Carl Gritter. This project is funded by the National Science Foundation and, to a lesser extent, by CAPO.

D. *Geometric Domain Processors*. This is a subproject of CAPO with the goal to produce two domain processors (2D and 3D) which handle general shapes. The construction is to couple only loosely the processing with the domain definition so that

ELLPACK EVOLUTION

A. BROADEN SCOPE

- EQUATIONS
  Increase the domain of applications handled
- DOMAINS
  Increase the number of domains used, allow more general 3D & 4D shapes

B. PARALLEL/DISTRIBUTED ELLPACKS

- VECTORIZATION
  Exploit the Cray, Cyber 205, etc. architectures
- PARALLELISM
  Use parallel algorithms in modules, replicated ELLPACK on a parallel machine
- DISTRIBUTED COMPUTINNG
  Access multiple machines with ELLPACKs. Reorganize ELLPACK into a distributed problem solving system

C. INCREASE ALGORITHMIC POWER

- NEW MODULES
  Add to the variety of methods available
- SOFTWARE INTEGRATION
  Provide good access to other large software systems

D. USER INTERFACE

- INTERACTION
  Provide modern computing environment
- SPECIALIZATION
  Provide front ends for particular application areas
- EXPERT ASSISTANCE
  Provide help with all phases of the computation

Figure 1. Overview of the potential directions for the evolution of the ELLPACK system. More detail is given in Figures 2A to 2D.

A. BROADEN SCOPE

EQUATIONS

- SIMULTANEOUS PDEs
  Many applications naturally involve a small system of PDEs
- HIGHER ORDER
  the stress/strain properties of materials require 4th order PDE models
- NONLINEAR
  Many phenomena are inherently nonlinear in the equations, boundary conditions or variable coupling
- TIME DEPENDENT
  A real world fact
  - PARABOLIC
    Important and closely related to ELLPACK capabilities
  - HYPERBOLIC
    Requires a complete new set of capabilities

DOMAINS

- MULTIPLE DOMAINS
  Many applications naturally involve distinct domains
- DOMAIN MAPPINGS
  Changing variables (and domains) is a powerful problem solving tool
- GENERAL 3D SHAPES
  General 3D shapes are important, we can't wait until all the shape problems are solved

Figure 2A. More detail of the potential directions to broaden the scope of ELLPACK.

B. PARALLEL / DISTRIBUTED ELLPACKS

VECTORIZATION

Various modules within ELLPACK are vectorized. Machine specific versions are created. First priority is in SOLUTION modules, then DISCRETIZATION and OUTPUT

PARALLELISM

- ALGORITHMS
  Various modules are developed suitable for machines like the NCUBE, SEQUENT, etc. Machine specific versions of SOL., DISC. and OUTPUT created.
- MULTIPLE ELLPACKS
  Copies of a slightly modified ELLPACK are used on a homoegeneous parallel machine to implement domain decomposition strategies.

DISTRIBUTED COMPUTING

- MULTIPLE MACHINES
  Access to ELLPACK systems on different machines is provided and the machine selected is that most appropriate for the problem.
- DISTRIBUTED PROBLEM SOLVING
  The ELLPACK system is reorganized into a set of compatible but independent problem solving modules. These are then available through a network of machines and implementations.

Figure 2B. More detail of the potential directions of evolution of ELLPACK into parallel and distributed computing.

C. INCREASE ALGORITHMIC POWER

NEW MODULES

- MULTIGRID
  A powerful new method only
  weakly represented in ELLPACK
- CONJUGATE GRADIENTS
  Completely missing now,
  probably of value
- SPECTRAL METHODS
  Of uncertain value,
  surely good at times
- A POSTERIORI ERROR ESTIMATOR
  A very valuable tool, probably
  practical to do
- ADAPTIVE ALGORITHMS
  Powerful methods weakly
  represented in ELLPACK
- BETTER DISCRETIZATION
  New basis functions for collocation,
  higher order finite differences for
  general domains, singular elements,
  etc., are all of value.

SOFTWARE INTEGRATION

- SYMBOLIC SYSTEMS
  Access to MACSYMA or
  REDUCE wold greatly aid
  a number of ELLPACK tasks
- STRUCTURES SYSTEMS
  One might add a lot
  of capability here without
  recreating a large system.
- CAD SYSTEMS
  Practical access to a
  CAD system would increase
  geometric flexibility
  greatly.
- OTHER PDE SYSTEMS
  One might add time
  dependence and other
  facilities more easily
  this way

Figure 2C. More detail of the potential directions to increase the algorithmic power of ELLPACK. The software integration possibilities also broaden the scope of ELLPACK.

D. USER INTERFACE

INTERACTION

The computing power is available and users should demand it. Color graphics workstations are used and some portability lost.

SPECIALIZATION

Front ends that focus the context of ELLPACK on a particular application area can greatly ease the use of such a complex system problem.

EXPERT ASSISTANCE

- ADVISOR SYSTEM
  Guides user through possibilities for using ELLPACK on his problem. Result is, at most, a preliminary ELLPACK program for his problem.
- EXPERT PROBLEM SOLVER
  Guides user through the whole problem solving process, helps him select, change and evaluate methods or results.
- MACHINE SELECTION
  Guides user through selection of appropriate machines. May be fully automatic.
- AUTOMATIC PARALLIZATION
  Helps partition the computations and allocate the tasks within a multiprocessor.

Figure 2D. More detail of the potential directions to develop better user interfaces for ELLPACK.

a variety of geometric representations can be used. Data structures are defined for 3D objects which make later phases of problem solving easier. This working by Bajaj, Cui and Rice.

E. *Parallel Algorithms for PDEs.* There is AFOSR support to develop parallel methods for PDEs. The focus (from the ELLPACK point of view) is on developing new modules for DISCRETIZATION and SOLUTION. Several algorithms have been developed and a couple implemented as ELLPACK modules. Work in this general area is also supported by CAPO and the work is not tightly constrained to heavily involve parallelism. The faculty involved are Houstis and Rice with support from post-docs M. Vavalis and Mu Mo plus several graduate students.

F. *Distributed PDE Systems*. Work in this area is supported by CAPO, by the above AFOSR project and by an ARO grant on Advanced Parallel Systems. The aim is to develop both "distributed PDE solving techniques" and massively parallel algorithms. Thus there is considerable overlap with the proceeding project. A number of theoretical papers have been written and the first steps are being taken to implement usable software for controlling parallelism.

6. GOALS, CONSTRAINTS AND PRIORITIES

In this section we outline the general goals of ELLPACK evolution and the constraints imposed by funding (both resources available and topics to be emphasized). From these we derive some general priorities but the specific tasks and plans are still very open within these priorities.

A. *Goals*. The following general goals come from the nature of a university environment, association with other projects and personal preferences.

1. *Innovation in Design and Capabilities*. We want something that keeps us at the forefront of developing sophisticated scientific computation systems.
2. *Demonstrate Feasibility*. We do not want a paper system, it has to be believable that a really good, production quality system can be built.
3. *Useful System*. The system has to be capable enough to meet some needs of the CAPO project. It would also be very nice if independent use can be made of the system.
4. *Framework for Research Results*. There must be ways for a variety of narrowly focused research projects to be fit within the overall plan.
5. *Prototype Available in 1-2 Years*. By 1990 we must be able to show something that demonstrates real progress.
6. *Enhanced Modularity*. We strive to interface with various groups, projects and software systems. ELLPACK is already modular in many ways, but further steps are needed. In particular, better separation is needed between domains (geometry), equations, methods and the specific user interface.

B. *Constraints*. We must fit within the scope of projects that are funding the work. That presents little problem with CAPO as almost everything envisaged could be useful there. The current AFOSR and ARO grants are focused on parallelism in scientific computing, preferably massive parallelism. They also focus on scientific applications (which presents no problem). The NSF grant of Dyksen focuses on user interfaces and the ARO/ONR grant of Bajaj focuses on geometry.

The level of support availble is currently fairly good and should improve some in the future. Nevertheless, there is *much less* available than needed to do a good job in many (never mind all) of the potential directions. The resources available are listed.

Equipment. Currently have good color graphics workstations, an Alliant, a 128 node NCUBE, access to a Cyber 205 and to a good UNIX server. Funds for more workstations, upgrading the NCUBE to 256 processors and further enhancements are very likely to become available. We conclude that equipment is not likely to be a problem.

Faculty. Currently Bajaj, Dyksen, Houstis, Lynch and Rice have some involvement in this area. There are no current prospects for more faculty and some of these people have other, somewhat unrelated, commitments.

Post-Docs. Currently E.A. Vavalis and Mu Mo are involved in this area and will be for at least a year or so more. Prospects for continued and even increased support are good, but post-doc positions are financially uncompetitive and thus hard to fill.

Graduate Assistants. Currently Bonomo, Cui, Christara, Chrisochoides, Gritter, McFaddin and Samartzis are involved in some way with such projects. Support for 6-8 research assistants seems likely for the next few years but one must keep in mind that some may go in other unrelated directions or become deeply involved in thesis projects that make no direct contribution.

Professional Programmers. There is some assistance now for keeping the general systems going. More is expected in the future but one cannot count on having a talented, knowledgeable person dedicated full time to this project.

Figure 3 shows the priorities that are derived from these considerations and which seem plausible with the resources envisaged. The scale uses the following grades:

A: Something must be accomplished or the project will not reach its goals.

B: Attractive directions but not absolutely essential that a lot be done.

C: Nice things to do, but not really needed in the current environment.

EVOLUTION PRIORITIES

A. BROADEN SCOPE

- EQUATIONS
  - 2yr: **A–**
  - 4yr: **A+**
- DOMAINS
  - 2yr: **A–**
  - 4yr: **A+**

B. PARALLEL/DISTRIBUTED ELLPACKS

- VECTORIZATION
  - 2yr: **C**
  - 4yr: **B**
- PARALLELISM
  - 2yr: **A**
  - 4yr: **A+**
- DISTRIBUTED COMPUTING
  - 2yr: **B+**
  - 4yr: **A**

C. INCREASE ALGORITHMIC POWER

- NEW MODULES
  - 2yr: **C**
  - 4yr: **B**
- SOFTWARE INTEGRATION
  - 2yr: **B**
  - 4yr: **B+**

D. USER INTERFACE

- INTERACTION
  - 2yr: **A**
  - 4yr: **A+**
- SPECIALIZATION
  - 2yr: **C**
  - 4yr: **C**
- EXPERT ASSISTANCE
  - 2yr: **B+**
  - 4yr: **A+**

Figure 3. General priorities for the potential direction of evolution of ELLPACK. The grades given for 2 year and 4 year time frames are: **A** = essential, **B** = not absolutely essential but very desirable, **C** = desirable.

APPENDIX: ELLPACK LITERATURE

This does not include publications primarily about the numerical methods used in ELLPACK modules.

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