COMPUTATIONAL COMPLEXITY IN MULTIDIMENSIONAL
NEUTRON TRANSPORT THEORY CALCULATIONS

Progress Report

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NEUTRON TRANSPORT THEORY CALCULATIONS

Contract No. AT(11-1)-2280

Project Abstract

The objectives of our research remain the same as outlined in the original proposal. They are in short as follows. Develop mathematically and computationally founded criteria for the design of highly efficient and reliable multi-dimensional neutron transport codes to solve a variety of neutron migration and radiation problems. Analyze existing and new methods for performance.

To achieve our goal we have subdivided the problem into three major steps:

Step 1: Automated error analysis over computational cells.

Step 2: Global error and stability analysis.

Step 3: Systems analysis and assessment of computational efficiency.

Each of these steps consists of three parts.

- a.) Rigorous analysis of the analytic behavior of the mathematical solution for any sub-problem.
- b.) Implementation of computer codes. Generation of representative benchmark problems for which the exact solutions are known.
- c.) Evaluation of test results and recommendations.

Scientific Background

In the original proposal we have a condensed seven page history on the development of transport theory calculation techniques. From this summary, it becomes clear, that the original transport theory calculations started with the solution of the half-space problem (the Milne problem), then progressed to calculations in slab, spherical, and cylindrical geometries. As the sophistication in nuclear reactor design increased, two-dimensional transport codes in (x,y)-geometries were demanded and designed. The numerical methods used in these codes were generalizations of the techniques applied to one-dimensional geometries, namely linear approximations in the space-variables and spherical harmonics or linear and nonlinear discrete ordinate methods in the angular direction.

Contrary to a widespread view, many of these codes have a solid mathematical foundation for their intended use. However if the mathematical assumptions underlying the implementation of these codes were to be satisfied, the cost of computation would become prohibitive. Besides this argument a great deal of ingenuity and hard work went into data management. A typical core design starts with a 1000 group calculation with subsequent group collapsing. However, very few researchers bothered to analyze the behavior of the mathematical solution to the given problem. Thus, with the present approximation methods and convergence criteria used, no assurance for a correct answer with a predetermined error estimate can be given. For a simple mathematical and graphical visualization of this point, the reader is referred to Appendix A of last year's proposal, to Appendix B of report C00-2280-17 pp. 133-150 (November 1974), as well as to Figure 4 (page 22) of the enclosed report C00-2280-21.

How different numerical results can be, is shown by the following example. We solved the neutron diffusion equation

$$-\nabla D \nabla u + \Sigma_a u = S(r, \theta) \quad u = u(r, \theta)$$

in an infinite circular cylinder with reflecting boundaries that contained two regions in the form of wedges with the common vertex on the center line of the cylinder (center of the corresponding two-dimensional disc). The coefficients D , Σ_a , and the source S are regionwise constant. Using the dimensionless form of the above equation, we obtained with the finite element method the flux profiles as indicated in Figure 1. Using slightly fewer node points and a finite difference scheme for the same problem, the flux profiles are indicated by Figure 2. (Note that in the notation in the Figures we made use of the symmetry properties of the problem). The interesting fact is that by adding just one extra node on the circular boundary in Figure 1, at the "right place," we can obtain a positive flux. We made a series of such calculations, and the above cited example is quite representative. Similar statements can be made for the numerical solutions of the two-dimensional transport equation.

A scientific approach to solve such discrepancies in numerical solutions is to obtain exact (analytic) solutions to simple benchmark problems (as exemplified) and then compare these with the results of different numerical methods. Since exact solutions in two-dimensional multiregion problems are (almost) impossible to obtain, the next best step is to study the analytic behavior of the solution where singularities are expected and then manufacture benchmark problems which represent the real situation. This is a basic point of view which we adopt in our research. Figure 3 represents the result of such an attempt for the

Figure 1

FINITE ELEMENT METHOD

S(2) = 0.
 S(1) = 256.0000
 C(2) = 256.0000
 C(1) = 256.0000
 D = 4.0000
 ALPH = 45

Figure 2

FINITE DIFFERENCE METHOD

S(2) = 0.0000
S(1) = 256.0000
C(2) = 256.0000
C(1) = 256.0000
D = 4.0000
ALPH = 45

Figure 3
SERIES EXPANSION METHOD

S(2) = 0.
S(1) = 16.0000
C(2) = 16.0000
C(1) = 16.0000
D = .2500
ALPH = 60

diffusion equation. A glance at the angular flux profile shows that the answer is not quite satisfactory. The reason is that the calculations for Figure 3 are very expensive compared to our other calculations described below, and we were not willing to invest more money in computer time. However, we can use this solution to manufacture a benchmark problem with known exact solution, that approximates the original problem.

We shall conclude this brief exposition of the scientific background by referring to the list of publications supported under this contract, where detailed information can be found. Note that items 1 through 15 have been submitted previously, item 16 and 17 are enclosed with this proposal.

Scientific Scope

As we pointed out previously, our aim is to develop a theory of error estimation for coarse network calculations in neutron migration problems and implement the results simultaneously in a computer code for use by engineers and scientists that are not specialists in numerical analysis. Simultaneously, new numerical methods are developed and tested. The approach requires a rigorous, systematic approach, and implies a great amount of theoretical and development work, which will not be visible to the average user in the end product, the systems code. We try to look at the problems from all angles and then make a best selection for the implementation in the code.

We cooperate with the Nuclear Engineering and Applied Mathematics Committees at Northwestern University, the Applied Physics and the Applied Mathematics Divisions at Argonne National Laboratory, as well as with other Laboratories and Universities in the U. S. and abroad. All work involves participation of graduate students. The project forces the students to thoroughly understand the basics of applied mathematics, and to translate new mathematical theorems into working computer codes. Judging from the past record, both government and industry employers seem to be impressed by their training as evidenced by the students' employment compensation.

Work Accomplished

Although the main portion of the research is accomplished during the summer months, a good part of the work proposed in last years' research contract has already been accomplished, and we believe that we will be able to produce the remainder by August 31, 1975 with minor exceptions. We list our accomplishments in reverse order of last year's proposal.

"On Hopf Type Maximum Principles for Convex Domains."

The principal investigator of this part of the project was Ivar Stakgold. The results are reported in the enclosed progress report C00-2280-20 with the above mentioned title.

In the simplest nonlinear model of a reactor, the neutron density satisfies the nonlinear Dirichlet problem

$$\Delta u + f(u) = 0 \quad \text{in } D, \quad u = 0 \quad \text{on } \partial D.$$

We have been concerned with estimates for such quantities as the gradient of the solution, the mean-to-peak ratio and other global measures of the effectiveness of the reactor. These estimates have been obtained by the use of the Hopf maximum principle for elliptic differential inequalities. In the most recent work a sharper maximum principle has been derived which yields improved bounds for both the nonlinear and linear cases. For instance we have been able to show that for the principal eigenfunction of $\Delta u + \lambda u = 0$, $u=0$ on the boundary, the following inequality holds

$$|\text{grad } u| \leq \sqrt{\lambda} \left\{ \left[1 + \frac{k_o^2}{4\lambda} \right]^{\frac{1}{2}} - \frac{k_o}{2\sqrt{\lambda}} \right\} u_M,$$

where k_o is the least average curvative of the boundary (assumed convex).

Dr. Stakgold will leave Northwestern University at the end of July 1975. If time permits, a second report will be submitted.

Improved Error Analysis Package

The enclosed progress report "Quantitative and Computerized Error Analysis" C00-2280-21 describes the Error Analysis Package BEAPAC-1T, coded in FORTRAN for the IBM 360-195 system. It is an improved version of BEAPAC-1T for the CDC-6400. The following changes have been made. It is a strictly modular system, with all algorithms accessible as sub-routines. The numerical methods which are part of BEAPAC-1T, are reduced to the matrix form $Ax=b$. This permits an easy comparison of the different numerical methods, but also reduces computer time. To generate a benchmark problem, solve the transport equation for twenty different mesh configuration, determine the absolute maximum error in the flux,

print a summary table, such as Table 1 of the enclosure, and plot the exact solution costs from 3 cents to 14¢ at the Argonne National Laboratory IBM 360-195, depending on the priority. If in addition 20 error plots such as Figure 3 of the enclosure are desired, the total cost ranges from 20¢ to 85¢. The system permits also to be interfaced with an existing transport code, if the matrix form $Ax=b$ of the corresponding algorithm has not yet been determined or added to the system as a subroutine. Another addition is the Mode Analyzer. If a numerical solution is given, a benchmark problem can be generated from a set of the regular and a new type of eigenfunctions that approximates the given solution. For this generated benchmark problem, an error analysis can be performed by the computer. Furthermore, two-cell benchmark problems can also be generated. This latter capability was introduced ahead of time, since it was requested repeatedly by the engineers and physicists with whom we consulted.

An obvious contender for a new numerical approximation method for the transport equation is the expansion of the flux in approximate asymptotic and transient eigenfunctions used in the mode analyzer.

A CDC-6400 version of this code will be used by another group at Northwestern University in an NSF sponsored project which investigates in particular the interface current technique (also known as response matrix method or transmission probability method).

Two-Dimensional Benchmark Problems

The Benchmark Error Analysis Code for two space dimensions will also be able to evaluate numerical methods for solving the neutron diffusion equation. This addition is made because we feel that we can extend the usefulness of the code considerably at only nominal cost.

We concentrated on the benchmark problem described in the section "Scientific Background." The physical setting is a two-dimensional neutron migration problem over a circular disc with reflecting boundaries. The domain consists of two wedges with different material coefficients (see Figures 1 to 3). This simulates a corner problem, where we can study the singular behavior of the mathematical solution. We choose the Neumann problem (instead of Dirichlet problem) because the reflecting boundary simulates the connection of the solution with the remainder of the nuclear reactor. The circular disc cuts out a finite neighborhood of the corner. For such a small problem, one can attempt to obtain an analytic solution in a series expansion. A parameter study of the actual numerical solutions for a bounding set of material constants gives a quantitative knowledge of the importance of the different terms in the expansion. For the neutron diffusion equation, the results for the two-wedge problem are reported in C00-2280-14, "The Interior Corner Problem for the Neutron Diffusion Equation." In this report, which uses the "traditional" approach, it is shown that the obvious generalizations of the results concerning the Laplace and Poisson equations as reported in the literature are misleading. The elements of a new theory are also given that show how to use the analytic solution to predict success or failure of an approxi-

mation methods for coarse network calculations.

In item 24 of the publication list, we were able to derive at a transport theory integral equation for the scalar flux for the same problem as above. The solution of this equation gives quantitative insight on the validity of replacing transport theory by diffusion theory in practical applications for corner problems. The derivation of the kernel for the integral equation is by no means trivial, and cannot be summarized in a short paragraph. In the corresponding code, we have still some computational difficulties.

Characteristic Theory of the Transport Equation in Phase Space

The work is an expansion of our original ideas expressed in report C00-2280-1. We are able to present a simpler structure for our previous result.

Work to be completed by August 31, 1975

We hope to finish the work on the four reports item 21 to 24 of the publication list. There will be a symposium on sparse matrices at Argonne National Laboratory in September 1975 which we intend to attend. The manuscript (item 20) will therefore be held for possible additions and improvements.