COMPUTATIONAL COMPLEXITY IN MULTIDIMENSIONAL
NEUTRON TRANSPORT THEORY CALCULATIONS

Progress Report

MASTER

Erwin H. Bareiss

Northwestern University

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Technical Program

Objective: 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 theory codes to solve a variety of neutron migration and radiation problems. Analyze existing and new methods for performance.

Strategy: 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.

Historical Remarks and Reason for the Proposed Research

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.

As 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 becomes 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 visualization of this point, the reader is referred Appendix A).

How different numerical results can be, is shown by the following example. A very well-known two-dimensional discrete ordinate code

produces "ray effects" in a region with corners, i.e. very well-defined ridges in the scalar flux. A great number of papers have been written and many suggestions were made on how to smooth these numerical results so as to obtain the solutions "which the engineer expects". Then Northwestern University implemented a Finite Element Transport Theory Code which produces "smooth" solutions. This event prompted a prominent speaker at a national ANS meeting to declare that only in FEM is hope for further progress in transport theory calculation techniques, disregarding the fact that equally smooth solutions can also be obtained by low-order spherical harmonics solutions. The scientific approach to solve such discrepancies is to obtain exact (analytic) solutions to simple benchmark problems 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.

We shall try to describe the behavior of the solutions of the transport equation in simple terms, namely in terms of optics. If we have a monochromatic light source, then the transport equation is also used to calculate the diffusion of photons in an absorbing and/or scattering medium. Obviously, in the vacuum, the equation reduces to the theory of geometric optics. Thus, if an object is placed in a light beam (read neutron beam) in the vacuum, we will have a shadow

effect; and (partial) reflection, (partial) transmission, and (partial) absorption within the object. Obviously, the behavior of the solution is very singular. This oversimplified situation represents void calculations in a nuclear reactor, (void calculations are used to predict the escape density of neutrons at control and fuel rod openings at the surface of a reactor.) On the other hand, if the light beam hits a highly absorbing flat piece of material, the light beam will diffuse and its density will decay exponentially. This situation represents shielding calculations in neutron transport. In the core of the reactor with its complicated detail structure, we have singularities at each interface and edge of a material change. Computationally, these singularities are very difficult to treat. So far, all production neutron transport codes have ignored this singular behavior. In one-dimensional calculations with smooth geometries (slab, sphere) and linear space and angular discrete ordinate approximations, these computational difficulties are no problem. However to try to reduce the number of spatial meshpoints by using high order polynomial approximations and disregarding these singularities is a wasteful effort. In particular, it is wrong to keep a certain mesh configuration fixed, increase the order of polynomial approximation and conclude that this sequence converges to the exact answer. (See Appendix A for a simple example.)

We have asked a number of experienced transport theory code users what accuracy they obtain when comparing the calculated results with experimental data. For fuel modification in fast experimental reactors the answer was 5 to 10 percent, for shielding calculations,

the answer was about 30 percent, while void calculations are so unsatisfactory that no percentage estimate was given. Obviously, a great part of the error is due to the experimental data itself. For this reason, we are not convinced that improved transport theory calculations can reduce these percentage figures by a factor of 10, although in certain cases the users indicated they need results which are accurate within 1/10 of one percent. However, all persons questioned remarked that they would like to have three-dimensional transport codes. Surprisingly enough, no one complained over the high cost of the computations. Compared to the total cost of the experiments, computing costs seem very small. There is however a certain uneasiness about the reliability of the transport theory calculations. From this practical point of view, it seems most desirable to build transport theory codes on a sound mathematical foundation with a reliable formulation of the error estimates. In particular, since influential government officials have expressed a fear of breeder reactors, the least we can do to help overcome the energy crisis and assure our own safety is to furnish the reactor designers with trustworthy mathematical algorithms.

Relationship to Similar Research Efforts

If we consult the literature, there is visible a continuous effort to improve existing and design new and more efficient and reliable neutron transport codes. This is also one of our aims. The general procedure is to publish a method, implement it in a code, and demonstrate that it is superior to another code by comparing some numerical computations. As we have seen, the numerical values under

consideration are very rarely compared with the exact mathematical solutions. Our approach is as follows:

(1) The research is directed toward developing a classification of transport theory codes that permits an ordering with respect to reliability and efficiency of the underlying methods.

(2) The goal is to design a method of error analysis that is applicable to large mesh sizes or large finite elements, and to have the computer do this error analysis. The traditional method has been to show only that the error behaves like $O(h^s)$ as $h \rightarrow 0$.

(3) The global analysis is based on the performance and reliability of elementary cell calculations. (These calculations are inexpensive.) In other words, we try to use a systematic method to find the weakest link in a chain of algorithms and to replace it by a stronger one.

(4) We simultaneously try to establish the true analytic behavior of the mathematical solution of the problem.

A basic question is how to generate benchmark problems. Our approach has been to use the eigenfunctions or combination of eigenfunctions as presented in the original proposal to generate exact solutions to benchmark problems which produce in general a zero source term. Since we have shown that our extended set of eigenfunctions forms a complete system, they can be combined to form solutions to problems which represent the actual behavior of real problems. We find the "eigenfunction approach" a natural but not necessary way to set standards for benchmark problems. This is enhanced by the fact that the absence of a source term does not influence the mathematical theory of error analysis at this level

of testing. It should be emphasized that the general method (and the package of subroutines we produce) can be applied to other linear equations, such as the Poisson equation, Helmholtz equation, wave equation, integral equations and others. Its application to the transport equation is of greatest importance since the mathematical complexity of the multi-dimensional problems is comparable to that of the hydromechanics equations, but the mathematical theory is still underdeveloped and known analytic solutions are non-existent.

A particular simple class of operators for which our approach is very well suited are matrices. Since matrices, through their Jordan canonical form, have a well-defined structure, it is possible to generate exact benchmark problems by similarity transformation. The basic transformation matrices are unit triangular (sparse) matrices which can approximate any given condition of the eigen and principal vectors. (For a more explicit description, we refer to Appendix B). We note that matrix analysis is an integral part of our stability and complexity analysis of numerical methods to solve neutron transport problems. As the reader recalls, the NATS Project, sponsored by NSF and AEC, has the purpose to test matrix routines for their reliability. About 30 matrices with known condition numbers were chosen to test matrix routine for performance. The shortcomings of such a procedure, though very valuable, has been recognized by the University of Illinois and Argonne National Laboratory. At this moment it is planned that, with our cooperation and that of the University of Illinois, Argonne National Laboratory will implement a portable benchmark generating code which will enable any installation to test its own matrix routines.

Furthermore, as of this moment, the Applied Physics Division at Argonne National Laboratory expects to fund a benchmark project for transport theory codes. Argonne has offered the graduate student who wrote the prototype error analysis code, to complete his dissertation at Argonne under the Argonne-University cooperation plan. This is therefore a strong indication that the results of this research have practical value.

Work Accomplished

The work accomplished in our first reporting period is summarized in Progress Report C00-2280-3. Basically, we constructed and applied a prototype error analysis code for one-dimensional neutron transport codes, that can generate benchmark problems for computational cells and furnish the actual error in graphic form as well as in tabulated form for different types of error norms.

This reporting period saw again a very lively activity. The project is credited with 8 reports and papers that are either completed, accepted for publication, or published. In addition, there are 3 drafts of manuscripts completed which need final editing before release and 3 reports are in preparation. These reports are listed at the end of this section. Although we feel we have more than satisfied the requirements of the contract at this time, we regret the delay in issuing some of the reports and research results. This is due to the fact, that the principal investigator carried a full load of teaching, besides supervising, counseling, and advising in research.

We discuss briefly the progress made in the different areas of our research during this fiscal year.

An important part in testing numerical methods is to investigate

their performance in approximating the transient part of the transport theory solution. Such solutions are given by linear combinations of the generalized eigenfunctions, which in the one-dimensional case means integration of the eigenfunction, weighted with selected Fourier coefficient functions over the continuous spectrum. In our original proposal we considered only the weight δ which led us to the definition of the "rigged modes". A natural extension is to assume that the coefficient function can be approximated by a polynomial or rational function in the argument v of the integral, say v^k , or v_+^k , and so on. An example is given in Appendix C which represents well the solutions near interfaces.

We have also exposed our summary tables and graphs to criticism. While the graphs are readily accepted, our multiple entry tables were more criticized than praised. Our original idea was to pack a table with a maximum of information. However, many engineers seem to find such tables hard to read. We decided therefore to split the tables and make them as simple as possible without insulting anyone's intelligence. We reached also another practical decision. Our original intention was to create one code with an open-ended set of options that would do "everything". However users who have to study such a code get easily overwhelmed or confused. It appears that producing a package of subroutines that does exactly the same thing, is more appealing to the user. The user has the feeling he needs to learn or understand only one item at the time. Therefore, this approach seems psychologically the correct one. Hence we question whether the report by Derstine et al. (which is really a

finished product) should be released for general distribution because it describes the original thinking of implementation. We anticipate that by the end of the summer we have a prototype "2-dimensional" package ready for internal testing.

Considering the global aspects of transport codes, we are confronted with inverting sparse matrices. There exists a large literature on sparse matrices and graph theory, but there does not exist an introductory book that unifies the theories and uses the language of the numerical analyst. We have made an intensive literature search, and introduced many elucidating examples in the hope that the rather large report "Direct Methods for Sparse Matrices" will fill the void. Because we think this report will be of general interest, and the authors spend some time working on such problems at Argonne, it is intended to publish it as an Argonne National Laboratory Report in order to give it a wider distribution.

Finally, multidimensional neutronics calculations will demand matrices of such a high order that iterative processes will be necessary for the numerical solution. The work done on iterative factorization methods can be used to order or classify most existing diffusion theory algorithms with respect to rate of convergence and thus also with respect to computational complexity. While the investigations are not complete, it is hoped that a similar statement can be made with respect to transport theory algorithms.

The analytic behavior of the solutions of the diffusion and transport equation at corners and edges are also under investigation.

We simulate a simple realistic situation by considering a disc with segments of different, but piecewise constant material constants. The scalar flux has zero slope in radial direction (Neumann problem).

For the diffusion equation we obtain the exact solution in two different ways. In both approaches we use polar coordinates. In the first approach we expand the solution in a double series, a Fourier series in angular direction and expansion in Bessel functions in the radial direction. This is the classical approach that was also used by previous investigators. The difference is that we attempt to obtain the exact solution to the problem stated above. We are not satisfied with the $O(r^\alpha)$ approach; we want to determine the influence of the subsequent terms on the solution. In addition, we are interested in segments with vortex angles other than multiples of $\pi/2$. In particular, we are interested in vortex angles of $2\pi/3$ and $4\pi/3$. These calculations turn out to be extremely tedious. In the second approach, we use the integral equation form for the same problem. Here, our expansion starts with logarithmic terms. In our original proposal we mentioned the paper by Lehmann, on wedges, in which logarithmic terms appear and disappear as the vortex angle becomes an irrational or rational fraction of 2π . From a computational point of view such a behavior is very unsatisfactory and must be reconciled. Similarly, the expansion of the scalar flux obtained from the integral equation form of the transport operator contains logarithmic terms near the vortex.

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