COMPUTATIONAL COMPLEXITY IN MULTIDIMENSIONAL
TRANSPORT THEORY CALCULATIONS

Progress Report

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Abstract

The scope of this research is to develop highly efficient methods for neutron transport theory calculations. To achieve this goal, a method is developed to evaluate the reliability and effectiveness of existing and proposed new methods at low cost. The report summarizes the state of the present program and results already obtained, which promise significant savings of computation time and code development costs.

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Erwin H. Bareiss and I. K. Abu-Shumays

1. Basic Principles

A major tool for neutronic calculations in designing thermal and fast nuclear reactors is a set of diffusion approximation codes. However, in many instances, such as in shielding, void, fuel burn-up, safety and many more problems of importance to the government, transport theory calculations are required. These calculations were dominated in the past by what is known as the S_N -codes. In spite of their great utilization, shortcomings of these codes have been recognized early. Hence, over the years, many different approaches to transport theory calculations have been proposed. Certain isolated ideas were implemented in new transport theory codes when funding was available. Then the numerical solutions obtained by different codes were compared by defining arbitrary standards without analyzing the true mathematical solution of the problem (this being a very difficult task). In the past few years a trend set in to alter codes or methods, compromising rigorous mathematical reasoning, so that the numerical output conformed with the expectations of the engineer. While designing, by its intrinsic nature, will always remain an art, we adhere to the principle that supporting calculations should always be based on solid scientific ground. Therefore we conclude that a systematic performance evaluation of existing, new, or proposed transport theory codes is essential. Our work is based on a number of postulates.

Postulate 1., No evaluation procedure is best for all transport problems.

- Postulate 2. The user of a code is performance minded.
- Postulate 3. The user wants to set his own standards for performance.
- Postulate 4. Performance is measured by a ranking process according to specified criteria.
- Postulate 5. The union of all transport theory codes form partially ordered sets.
- Postulate 6. The set of all possible transport theory codes is open ended.
- Postulate 7. Visual aids are helpful in decision making.
- Postulate 8. Recommendation of a new approach does not imply that the previous methods are to be discarded.
- Postulate 9. Every evaluation procedure can be improved.

2. Economy of Code Selection and Development

Obviously, to run extensive tests on so-called realistic problems with different types of transport codes is very expensive especially since no absolute standards exist. However, the problem becomes manageable if the calculations are restricted to a very small representative set of model problems and then the global behavior of the methods is deduced. This is not only possible, it is necessary. For example, it is a tremendous effort to take all geometrical shapes of computational cells into account in multi-dimensional calculations. Of course, once such calculations are done, they can be collected in a suitable form for later reference. Indeed we plan to publish a collection of such cell calculations for a wide variety of approximation methods and geometrical configurations. But the main purpose of this collection will be to provide examples, illustrating how to use a computer code that will provide a performance rating for a specified calculation of a specified task.

The mathematical background for this code is given in Ref. 1, a short description of its use with sample outputs can be found in Ref. 2, and a more detailed description in Ref. 4. The basic ideas for the design of the code are as follows.

- a) Representative benchmark problems are generated for which the analytic solution is available to the computer.
- b) The benchmark problems are designed to test specific capabilities of the code that are necessary to perform a certain job.
- c) Only small scale calculations are necessary. As soon as a code with underperformance is detected, it is eliminated.
- d) A variety of options of performance criteria is available, and similarly options for output in tabular and/or graphic form are available.

The economy of this procedure is due to the fact that large scale computations for test purposes are eliminated, and even for small scale calculations, only the minimum amount of computation is performed. In addition, several codes or code variations can be run on one job dispatch to minimize the input overhead.

Similarly, if the objective is code design, only a part of the analysis over a computational cell may be sufficient to eliminate a method. This, of course, contrasts with the now prevailing custom of implementing any new method in at least a full one-group prototype code. In addition we should like to mention that certain capabilities of a multidimensional code can be predicted from one-dimensional calculations, and thus again, computer time can be saved.

3. Summary of New Results

Our research activities have been in the following areas:

a) Development of a prototype automatic error analysis code for one-, two- and three-dimensional problems as described briefly in section 2.

The present status of this code is more fully described in Appendix A and in Ref. 4.

b) Experimentation with one three-dimensional, four two-dimensional, and eight one-dimensional transport theory codes.

All codes, except the one-dimensional Finite Element Method code, should be considered new transport theory codes, since the approximation methods have not been published in the open literature. The methods are described in sufficient detail in References 2, 3, and 4. Evaluation of the numerical results of our experiments leads to the following important conclusion: The efficiency of a transport theory code depends critically on the appropriate relationship between the mesh width in space and the number of discretization nodes in angle. In other words, taking more space points (or angular points) than indicated by the optimum ratio does not improve the accuracy of the flux calculations; on the contrary, the accuracy may decrease. By not observing this new rule, the computing time may easily be two or four times as large as necessary. The importance of this observation is obvious if one considers an improvement of 20% in iteration time to be significant.

Comparison of the numerical solutions of the 1-D symmetrized self-adjoint transport equations indicates the following: The accuracy of the finite difference method (FDM) is on the average better by a factor of about 100 than the accuracy of the finite element method (FEM). This surprising result is discussed in Appendix B.

c) Analysis of boundary, interface and corner effects in two-dimensional transport theory calculations. We are of the opinion that efficient approximation methods to the transport equation can only be designed if we understand the analytic behavior of the mathematical solution of the problem. For this reason we investigated the influence of the add-on term $|x| \log|x|$ (x is along the normal direction to the interface or boundary), which is customarily neglected in all transport codes. The detailed results are described in Ref. 3. The conclusions are in summary:

With the presence of an add-on term $|x| \log|x|$ at boundaries or interfaces the number of mesh points can be reduced by at least a factor of two in a rather large neighborhood of the discontinuity without loss of accuracy in the net flux.

The presence of a corner in two-dimensional calculations causes discontinuities in the derivatives of the angular flux in the space variables and the azimuthal angle along the base characteristics emanating from the corner.

Compliance Statement

The principal investigator has spent considerable time on the project, but has not drawn any funds from the AEC grant except for two business trips. He expects to work full time and be supported by the grant during the summer. The co-principal investigator will be supported by the AEC grant half time during the remainder of the academic year and full time during the summer. Obviously, the work accomplished indicates that both principal investigators and their students have spent, percentage wise, much more time on the project than required by the contract. This was made possible by partial support from Northwestern University reflecting the cost sharing by the University. To our knowledge we have complied with all the terms of the contract.

Publications - References

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Appendix A: Automated Error Analysis Code

The code to be discussed here is the preliminary version of the automated error analysis code written after experience was gained from earlier applications of the normal mode solutions to the Hermite Birkhoff approximation, the 2-D and 3-D codes, and the associated programs to provide plotting and tabular data.

This code is an attempt to construct a convenient modular framework, within which an analyst can check out and compare approximation methods in a systematic manner at a minimum cost. Tabular and graphical facilities are already developed for immediate usage. A global loop structure is constructed for varying specifications on mesh, angle, mean free path, order of approximation and normal mode.

A number of options are currently available to suit the user's needs.

1. Convergence criterion: when selected, this option essentially allows only computations within the optimal band to be performed. Two extra elements are computed before the code considers a particular mesh or angle point to be outside the band. Since hindsight is necessary to detect the band, two successive increases in error prevent local fluctuations from distorting the picture.
2. Batch or Online(Interactive) modes are available from the single program. Thus the user may obtain immediate results. The Interactive mode has the capability of running via teletype or CRT and has a special feature for running via an Imlac PDS-1 graphics display terminal. The only advantage of the third capability at this time is immediate visual display of any graphical data. The Imlac, however, is equipped with a light pen, and possibilities for utilizing interactive graphics in

this code are many. Consider, for instance, the problem for finding optimal, finite elements in an irregular grid region.

3. Input is largely free-form: Data fields are separated by commas. Null data fields imply that the built in default value for parameters are desired. In Interactive mode, checkpoints are provided to enable the user to backup to the previous checkpoint and reenter data if an error is discovered.
4. Plotting options currently produce 3-dimensional error plots mapped to 2-D and produced in hardcopy form by a Calcomp Plotter. An independent code to produce three dimensional discretized function plots is working and will soon be added to the existing code.
5. The table generation option is currently designed to tabulate errors within a mesh angle framework. Four types are currently available. They are
 - (i) maximum absolute flux error at boundary nodes
 - (ii) maximum absolute flux error at interior nodes
 - (iii) maximum absolute flux error (both i and ii)
 - (iv) average global flux error

If the need arises the results may easily be summarized through minor additions to the program.

6. The error analysis currently computes maximum absolute signed errors for the angular and scalar flux at the nodal points of the approximation. The analysis distinguishes between errors on the boundary and in the interior of regions in order to observe the boundary behavior. The average of the absolute errors is also computed to provide a feeling for the variance of the error.

7. The user has the option of saving various crucial information on tape or disk files for further manipulation. In addition, the standard error summary data provides a means of restarting data runs in the middle of a large table run without having to rerun the entire job.
8. Dynamic storage requests in the matrix generator and solution overlay uses only as much central memory as needed. This item is not an option but is a design feature followed in the code.

In expectation of future expansion of the code a general overlay structure was constructed which allows a modular extension to each of the features of the code.

Appendix B: Solution of the Symmetrized Transport Equation

The derivation of the Vladimirov symmetrization process is described in Ref. 2. The symmetrized transport equation was solved for three sets of identical benchmark problems by finite differences (FDM) with Gaussian integration and by the finite element method (FEM) over phase space using the Lagrange functional. The Tables 3.6 and 3.7 of Ref. 2 summarize the corresponding results. Comparing the numerical results, the user concludes that FDM is superior to FEM and makes his selection. The mathematician sees a challenge: FDM used Gaussian integration, while FEM used an extremum principle. One would expect that the variational methods would minimize the error, so that both methods should be competitive. This is not so. However, if FEM would adopt non-conforming elements and place the nodal points at the discrete ordinates of the Gaussian integration, we conjecture that the results would be comparable. This example proves that FEM can be successfully challenged by FDM.