COMPUTATIONAL COMPLEXITY IN MULTIDIMENSIONAL
NEUTRON TRANSPORT THEORY CALCULATIONS
FINAL REPORT

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SUMMARY OF INVESTIGATIONS

The aim of this research was to establish a general method to assess the performance and reliability of computer codes for the numerical approximation of linear operators. The neutron transport operator was chosen as model, since it is fundamental to nuclear reactor and radiation calculations, leads to very large computational problems, and analytic solutions are not available for most practical problems. Where analytic solutions exist, the mathematical theory and formulation is complicated and their numerical evaluation is costly. /

Our general approach to solve the error problem is as follows. First, determine the mathematical behavior of the neutron flux at boundaries, interfaces, and corners (singularities) for physical situations of practical interest. Second, design a representative finite set of particular and homogeneous solutions which satisfy the transport equations exactly over a bounded, homogeneous domain, called a computational cell. Thirdly, make use of the linearity of the transport operators and employ some "tricks" to obtain exact solutions over the union of a set of contiguous computational cells. At this point we have an infinite set of Benchmark problems at our disposition which can be used to test existing transport theory (and diffusion theory!) codes for accuracy.

However, a user of an existing transport theory code may be interested only in his specific problem (called the ref-

erence problem) and the performance of his computer code. Hence to establish its reliability, he can create a "personalized" benchmark problem. To do so, he uses the free parameters of the general benchmark problem (which represents the existing mathematical singularities) and produces a function which approximates the solution of the reference problem in a least squares sense (which is accomplished by a Householder factorization). If the benchmark function differs from the reference solution more than the error tolerance permits, he extracts new input specifications for the user's code from the benchmark function and solves the new problem with the user's code. - Now, a comparison between the last numerical solution and the exact benchmark function, both of which are solutions to the same input data, clearly establishes the reliability of the user's transport code for this particular problem. More refined applications of the benchmark problems are obvious. The entire process to create personalized benchmark problems to given reference solutions and to perform a variety of comparison tests as indicated above, has been computerized (BEAPAC 1T and BEAPAC 3T).

Since a lot of mathematical thoughts went into the design of BEAPAC, the question arises whether a new and highly efficient numerical method can be devised by making use of the already existing subroutines which yield exact solutions to the transport equation without boundary conditions. (They form a subset of the base for the general solution space). Indeed, by satisfying the boundary- and interface conditions, as well as the source terms only in a least squares sense, we obtain the Boundary- and Interface Function Method for neutron

transport calculations. Although beyond the scope of this contract, a one-dimensional computer code was written which performed at least forty (40) times as fast as the standard transport codes for comparable error tolerance. A three-dimensional version is being developed.

Having made use of the mathematical properties of the solutions, the implementation of different algorithms leads always to the problem of efficient sparse matrix inversion or eigenvalue computation. We have considered the classification and stability of general iteration processes under the descriptive name Factorization Iterative Processes. Since neutron transport calculations may require matrices of order in the thousands, classic error bounds lead to very unrealistic results, in particular since many matrix systems derived from the transport equation are not positive definite. A natural problem therefore is to investigate a probabilistic error analysis of floating point computer arithmetic. In pursuing this new and not much theoretically explored objective, it became apparent that a central processor unit with constant relative difference (CRD) arithmetic would be more adequate for large scale computation. Also not in the scope of the contract, we investigated the advantages of such a computer and filed an invention disclosure (Case #S-49885) with DOE which is still pending.

For detailed information we refer to the forty reports and publications related to this contract. They are listed below and can be requested from the DOE Technical Information Center, P.O. Box 62, Oak Ridge, TN 37830.

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