The work supported by this contract addresses four basic computational difficulties that arise in the numerical simulation of neutral particle radiation transport:

1. Discretized radiation transport problems typically involve systems of equations with enormous numbers of unknowns. To reduce the number of unknowns and the resulting amount of computational effort, the development of methods that are accurate on optically coarse meshes has become a priority.

2. Iterative methods must be used to solve the resulting system of discretized equations, and the most basic iterative methods often converge very slowly. The implementation of faster iterative methods has been hampered by the mathematical complexity of transport problems, and difficult nagging issues of stability and robustness.

3. In complex Monte Carlo radiation transport simulations, the user must provide a great deal of input (i.e. biasing parameters) in order to make the simulation run efficiently. Luck, trial and error, and experience all contribute to the selection of adequate biasing parameters. As a result, the selection of these parameters can be a very time-consuming process.

4. The extension of current computational algorithms to ones that run efficiently on parallel-architecture computers has become a priority, in order to make optimal use of the possibilities inherent in parallelization.

The work accomplished under this contract [1-13] addresses each of these issues. In what follows, we will outline our results.

The development of advanced numerical transport methods that remain accurate for coarse spatial meshes requires mathematical techniques that enable one to predict theoretically how numerical schemes will perform in the presence of optically thick spatial grids. Such a technique is an asymptotic expansion that describes the evolution of transport theory to diffusion theory in an optically thick medium with small absorption. This kind of asymptotic expansion has long been known for the transport equation itself, but we have recently become aware that it can be applied to numerical schemes as well. Some of this work is described in [1] and [2]. [1] is a review article, discussing results that has been obtained in recent years. In summary, the use of this asymptotic expansion has enabled sound theoretical foundations to be laid for the use of certain types of differencing schemes. The predictions of this theory have, to this date, always agreed with detailed numerical calculations, and they have enabled robust methods to be implemented in
transport codes (at Los Alamos and Lawrence Livermore National Laboratories) and to be run confidently for problems that would probably have been unsolvable otherwise.

As explained above, there are two components to successfully developing an advanced transport numerical scheme: it must be accurate on coarse meshes, and it must lead to a system of equations that is easily solvable. Conventional iterative methods for discretized transport problems are often woefully slow. It is essential that rapid (acceleration) iterative schemes be developed to make the transport calculations as efficient as possible. We have treated this subject in [1] and [3-6]. In [1], we use the asymptotic expansion described in the previous paragraph to provide a stable acceleration method for a particular discretization scheme.

In [3-6], we develop a class of “quasidiffusion” methods that was originally suggested in the Russian literature. These methods involve formulating the linear transport problem in a nonlinear fashion that is accurate and amenable to a rapid, efficient, iterative solution. This particular way of approaching transport problems has major advantages, but some disadvantages. We have developed procedures that overcome some of the disadvantages. When this contract was terminated, this work unfortunately stopped. But, we believe that it has a great deal of promise and there are signs that LANL is beginning to take a renewed interest in it.

In [7-10], we have developed a completely different type of transport methodology that applies to Monte Carlo calculations. In the work described in the above paragraphs, we focused attention on deterministic transport calculations, in which the underlying transport equation is discretized in some specified manner and the resulting system of discretized equations is solved. In Monte Carlo simulations, individual particle histories are simulated using statistical (random number) procedures. In principle, there is no discretization process in Monte Carlo codes, and if one were able to simulate a given problem with an infinite number of histories, the statistical errors would vanish and one would obtain the exact solution. As a result, deterministic solutions have discretization errors but not statistical errors, and the opposite is true for Monte Carlo solutions.

The fundamental difficulty with Monte Carlo calculations is that they are often extremely slow. The sophisticated use of Monte Carlo codes involves the application of procedures that render the resulting algorithm unphysical in some way, but that nevertheless produces the correct answer with reduced statistical errors. To do this, biasing, or variance reduction schemes have been developed. When implemented optimally, these schemes enable Monte Carlo calculations to be performed at a small fraction of the computational effort that is required otherwise. However, the successful implementation of these biasing schemes requires that a large number of biasing parameters be chosen and optimized. At the present time, the code user is required to do this, and this effort can be very difficult and time-consuming.

In [7-10], we have developed and implemented a method in which the biasing parameters are determined automatically, by the computer code itself for 2-D multigroup transport problems.
The logic that underlies this method is conceptually simple (but algebraically complex). Conceptually, it is well-known that so-called zero variance methods exist. In such a method, one is able to generate one source particle, and this particle is guaranteed to produce the correct score at the (typically faraway) detector. Any other source particle will generate exactly the same score. Thus, the variance is zero, and in principle only one particle is needed to generate the answer. The trouble with this concept is that in order to implement it, one needs to know the exact solution of an adjoint transport problem, and acquiring this information is inevitably much more difficult than solving the original (forward) transport problem. So, zero-variance methods exist on paper, but they are impractical.

Our approach involves the implementation of a method that is patterned closely on the zero-variance method. The procedure is as follows: first, we formulate the adjoint transport problem needed in the zero-variance method and solve it deterministically, by discretizing the problem and obtaining the numerical solution on a grid. Second, using the (approximate) discrete adjoint solution, we calculate biasing parameters that are employed in the zero-variance method. (These parameters are approximate, because they come from a discretized adjoint solution, rather than the exact adjoint solution.) Third, the Monte Carlo calculation is run, using the deterministically-determined biasing parameters.

In [7-10], we carried out and tested this work in 2-D geometries. Our results showed that the concept was valid, and that it often produced results much more efficiently than codes using user-specified biasing parameters. In more recent work, done subsequent to the termination of this contract [11-12], we have extended this work to 3-D geometries and have performed a wide amount of testing. Our results are extremely encouraging; I have included [11] and [12] in this report because they demonstrate that the work begun under this contract has reached a very mature stage. Briefly, we have extended our theory to 3-D geometries and have compared the efficiency of the scheme to that of another automatic biasing scheme (AVATAR) developed at LANL. In nearly all of the problems that we have considered, the new Local Importance Function Transform (LIFT) scheme outperforms AVATAR, often by as much as an order of magnitude. Other issues must be addressed before the LIFT scheme can be regarded as fully operational; for example, it must be implemented with a continuous energy-dependent Monte Carlo code rather than a multigroup Monte Carlo code. However, there is very little doubt that this can be done without substantial effort.

The practical implication of this work is that with the new LIFT algorithm, Monte Carlo codes can become much more user-friendly and efficient. Code users will no longer have to endure a potentially lengthy trial-and-error process to determine biasing parameters. These parameters will be determined by the code itself - much more rapidly, accurately, and efficiently than the code user could hope to do by himself.
Finally, in [13], we have shown how a standard transport discretization scheme (not accurate on coarse meshes), combined with a rapid Diffusion Synthetic Acceleration (DSA) scheme, can be implemented efficiently on a parallel-architecture computer. The basic idea is to use a spatial decomposition technique: one subdivides the spatial domain of the problem into subregions, orders individual processors to solve the transport problem on individual subregions, and by communicating boundary information (across subregions) from one processor to another, one can iteratively solve the overall transport problem more efficiently.

In the DSA scheme discussed in [13], the transport problem is iteratively solved by first performing transport sweeps, and then by solving a diffusion equation that "corrects" the latest transport iterate. We have employed the concept of spatial decomposition for both the transport sweeps and the diffusion calculation. Our results demonstrate that the parallel version of the DSA scheme significantly outperforms the scalar version, depending on the nature of the problem. The larger the problem, the better the relative parallel-computer performance. This is completely to be expected; it is seen in virtually every other application of domain decomposition to parallel computer architectures.

In conclusion, the work accomplished under this proposal has been dedicated to the goal of developing advanced methods by which the numerical simulation of radiation, interacting with matter, can be performed. The simulation of radiation transport is essential in many problems of interest to the Department of Energy, and we hope that our work will enable such simulations to be performed with a significantly higher degree of accuracy and efficiency.
REFERENCES

Asymptotics & Acceleration:


Quasidiffusion & Related Topics:


Local Exponential Transform & Monte Carlo:


Multigrid & Parallel Processing:

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