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Title: Geometrically-Compatible 3-D Monte Carlo and Discrete-Ordinates Methods

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Geometrically-Compatible 3-D Monte Carlo and Discrete-Ordinates Methods

Jim E. Morel*, Todd A. Wareing, John M. McGhee, and Thomas M. Evans

Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). The purpose of this project was two-fold. The first purpose was to develop a deterministic discrete-ordinates neutral-particle transport scheme for unstructured tetrahedral spatial meshes, and implement it in a computer code. The second purpose was to modify the MCNP Monte Carlo radiation transport code to use adjoint solutions from the tetrahedral-mesh discrete-ordinates code to reduce the statistical variance of Monte Carlo solutions via a weight-window approach. The first task has resulted in a deterministic transport code that is much more efficient for modeling complex 3-D geometries than any previously existing deterministic code. The second task has resulted in a powerful new capability for dramatically reducing the cost of difficult 3-D Monte Carlo calculations.

Background and Research Objectives

There are two basic approaches for performing radiation transport calculations: deterministic and stochastic.[1] Deterministic methods are based upon a discretization of the Boltzmann transport equation together with a solution technique for the resulting discrete equations. Such solutions suffer from discretization error due to the approximate nature of the discretization procedure. The most popular deterministic method used in the radiation transport community is the discrete-ordinates (Sn) method.[1] Stochastic or "Monte Carlo" methods are based upon a computer simulation of the transport process.[1] In particular, individual particle "histories" are generated using pseudo random numbers in conjunction with source distributions and interaction probabilities. An estimate of the Boltzmann solution is obtained by averaging certain quantities associated with each particle history over all particle histories. In principle, Monte Carlo calculations yield exact solutions in the limit of an infinite number of particle histories, but with a finite number of histories, these solutions suffer from statistical errors. Deterministic methods tend to be more efficient than Monte Carlo methods if differential quantities are required, but Monte Carlo methods tend to be more efficient than deterministic methods if integral quantities are required. Monte Carlo calculations can be very inefficient if only a small fraction of the source particles actually contribute to the quantity of interest.

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Historically, transport calculations in complex three-dimensional (3-D) geometries have been almost exclusively carried out using the Monte Carlo method. This was initially due to the fact that deterministic methods required a prohibitively large amount of memory for 3-D calculations. However, in recent years it has been due to the fact that discrete-ordinates methods have been limited to rectangular meshes, which can be very inefficient for modeling complex 3-D geometries. The primary goal of this project was to address this deficiency by developing an algorithm for solving the neutral-particle discrete-ordinates transport equations on unstructured tetrahedral spatial meshes. Unlike rectangular meshes, unstructured tetrahedral meshes can be very efficient for modeling complex 3-D geometries.

The statistical error associated with Monte Carlo calculations can be dramatically reduced using variance reduction techniques.[1] There are many ways to reduce the statistical error in Monte Carlo calculations, but the only variance reduction techniques that do not require significant expertise and physical intuition on the part of the user are so-called "automatic" techniques. The MCNP code[2] is a highly advanced Monte Carlo radiation transport code developed at Los Alamos National Laboratory (LANL). The automatic variance reduction techniques used in MCNP require an "importance" function for each problem. The importance function in a region of phase space is proportional to the average contribution that a particle entering that region will make to the quantity of interest. Importance functions rigorously represent solutions to the adjoint transport equation.[1] Such solutions are usually obtained either using a deterministic transport code or a Monte Carlo algorithm such as the weight-window generator[2] in MCNP. Fortunately, a highly accurate importance function is generally not needed to significantly reduce statistical error. Thus one can generally perform a fairly crude deterministic adjoint calculation. The cost of such a calculation is generally much less than that which would be required to obtain an accurate deterministic solution to the original problem.

The secondary goal of our project was to modify the MCNP algorithm so that it could perform automatic variance reduction using an unstructured tetrahedral mesh importance function (adjoint solution) from our discrete-ordinates code. The existing capability used a deterministic rectangular-mesh code, THREEDANT,[3] to provide the importance function. The advantage of the tetrahedral-mesh capability is that even crude models of complex 3-D geometries are more efficiently generated with a tetrahedral-mesh rather than a rectangular mesh.

Importance to LANL's Science and Technology Base and National R&D Needs

Radiation transport is of fundamental importance in many fields such as nuclear reactor design and analysis, inertial-confinement fusion, health physics, medical physics, and nuclear weapons research. To the best of our knowledge, the tetrahedral-mesh code that we built was the first 3-D unstructured-mesh discrete-ordinates code ever developed. It gives LANL a unique capability for efficiently performing 3-D deterministic radiation transport calculations in complex 3-D geometries. We later give computational examples that demonstrate the effectiveness of our algorithm and associated code.

Scientific Approach and Accomplishments

Our first task was to discretize the transport equation. The discrete-ordinates method defines a particular angular discretization. These angularly discretized equations were discretized in energy using a standard technique known as the multigroup approximation.[1] We developed a tetrahedral-mesh spatial discretization scheme for these multigroup Sn equations using a finite-element approximation with a linear-discontinuous trial space . This completed the discretization process. Our fully discretized Sn equations were solved via the standard source iteration technique.[1] This technique consists of iteratively lagging the scattering source, and results in independent equations for the flux associated with each discrete angle and energy group. In principle, each of these flux equations can be solved via a lower-triangular matrix inversion once the unknowns have been properly ordered. This ordering is obvious on rectangular meshes, but it is not at all obvious on unstructured tetrahedral meshes.

Our next major task was to develop an algorithm for determining the ordering on such meshes. We successfully developed an algorithm for finding the lower-triangular ordering whenever it existed, but to our surprise, we discovered that the ordering does not always exist on unstructured tetrahedral meshes even though all of the terahedra are non-reentrant. It has long been known that any 2-D mesh with non-reentrant cells has a lower-triangular ordering for all of the flux unknowns associated with each direction. Thus we expected the same result for the 3-D case. Once it was determined that a lower-triangular ordering did not exist, we had to develop a technique for defining an ordering of the unknowns in spite of this fact. This ordering was done using graph theory.

Graph theory enables us to identify a set or "ring" of cells that are interdependent. Once such a ring is identified, the fluxes on one particular face of one cell are declared to be known at the latest iterative level, even though they are really known only at the previous level. This decouples the cells in the ring, allowing us to proceed with the standard

ordering algorithm. Fortunately, we have found that dependent rings are relatively rare, and when they do occur, they do not have a significant effect upon the performance of the standard source iteration procedure.

Our next major task was to develop a diffusion-synthetic acceleration (DSA) technique to speed up the iterative convergence of the source iterations. This is done by estimating the iterative errors after each source iteration using a diffusion approximation. These error estimates are then added to the transport iterate to obtain an improved or "accelerated" iterate. A classic difficulty with this method is that the diffusion operator must be discretized in a manner consistent with the transport discretization to avoid instabilities. The discretized diffusion equation consistent with the linear-discontinous spatial differencing of our discrete-ordinates equations has itself a discontinuous form. This is a non-standard form that results in a diffusion matrix that is not symmetric positive-definite. Because it lacks this property, the diffusion matrix equation is difficult to solve.

We circumvented this difficulty by generalizing a 1-D technique, originally developed by Wareing, Larsen, and Adams,[4] to 3-D tetrahedral meshes. The central idea of this technique is to approximately solve the discontinuous diffusion operator in the following manner. First one obtains a continuous and symmetric positive-definite diffusion matrix from the discontinuous diffusion matrix via a particular asymptotic approximation. Next one solves the asymptotic diffusion equation for a set of continuous error estimates. These continuous error estimates are then used to decouple the discontinuous diffusion equations in a manner that results in an independent 4x4 matrix for the discontinuous error estimates within each tetrahedron. Because each of these local matrices is so small, they can be efficiently solved using a direct technique to obtain the required discontinuous error estimates. Although this process does not produce an exact solution to the dicontinuous diffusion equation, it produces an approximate solution that is sufficiently accurate to result in effective acceleration of the source iteration process. This completes our description of the tasks that were required to obtain an unstructured tetrahedral-mesh discrete-ordinates algorithm.

Our algorithm was implemented in a code called ATTILA. To summarize, the main features of ATTILA include:

* discrete-ordinates angular discretization,
* unstructured tetrahedral mesh,
* linear-discontinuous finite-element spatial differencing,
* multigroup energy discretization,
* anisotropic scattering, and
* diffusion-synthetic acceleration of within-group scattering iterations.

The unstructured tetrahedral mesh allows for accurate modeling of complex three-dimensional geometries. The linear-discontinuous spatial differencing scheme is considerably more accurate than traditional diamond or weighted-diamond differencing schemes and allows for the use of relatively coarse meshes. The use of DSA considerably increases efficiency of the code.

To demonstrate the effectiveness of ATTILA, we consider a nuclear well logging problem. The problem is a model of a dual-detector neutron porosity tool that has been lowered into a borehole. The desired result is the ratio of the reaction rates from the two detectors. This ratio yields the porosity of the strata surrounding the borehole. The geometry is too complicated to describe here, but a complete description is given in Refs. 5 and 6. A grid containing 14,633 tetrahedra was used for this problem. A top view of the grid is shown in Figure 1, and a blow-up side view of that part of the grid containing the tool is shown in Figure 2. The ATTILA calculations used S4 level symmetric quadrature and P3 scattering. In Table 1, we compare the ratio of the detector reaction rates obtained from ATTILA with BUGLE-80 47-group cross-section data and from MCNP with continuous-energy cross sections.

Table 1. Comparison of ATTILA and MCNP results for the tool problem.

Code	Reaction Rate Ratio (near/far)	CPU Time (hours)
ATTILA	3.265	0.91 (on IBM RS-6000)
MCNP	3.269 (+/-) 0.99%	30.5 (on CRAY-YMP)

The results indicate very close agreement between ATTILA and MCNP. The MCNP calculation required about a factor of 30 more computing time than the ATTILA calculation, but the IBM RS-6000 computer is roughly twice as fast as the CRAY-YMP for non-vectorized code. Since neither ATTILA nor MCNP is vectorized, one would expect MCNP to require about 15 times more CPU time than ATTILA for this problem using one machine for both calculations. The MCNP calculation was carried out with automatic variance reduction using an importance function from the MCNP weight-window generator. Thus the comparison of CPU times is a fair one.

The ATTILA calculation with DSA took 497 inner iterations and a CPU time of 0.91 hours on a IBM RS-6000 workstation. The ATTILA calculation without DSA took 1691 iterations and 2.48 hours on a IBM RS-6000 workstation, clearly showing the advantages of DSA. Only a small number of groups have scattering ratios near unity. Acceleration significantly reduced the number of iterations for these groups, while having a

relatively small impact on groups with scattering ratios much less than unity. For instance, group 4 took 16 iterations unaccelerated and 12 iterations accelerated, whereas group 47 took 687 iterations unaccelerated and 26 iterations accelerated.

Our last major task was to modify the MCNP Monte Carlo code to use adjoint solutions from the ATTILA code for automatic variance reduction. This required the implementation of a tetrahedral-mesh ray-tracing algorithm in MCNP. This algorithm was obtained from the literature. Every time a Monte Carlo particle undergoes an interaction, the value of the importance function must be evaluated. Thus, given coordinates for a point of interaction, one must determine the tetrahedron within which that point lies. When a particle is first created, a costly global search over all of the tertahedra is required to determine the tetrahedron it lies within. However, because particles travel in straight lines between interactions, each subsequent interaction point can be efficiently mapped to the tetrahedron it lies within using a ray-tracing algorithm. Fortunately, this algorithm is much more efficient than the global search algorithm.

The automatic variance-reduction package within MCNP is called AVATAR. It uses either a deterministic importance function from a rectangular-mesh discrete-ordinates code or a stochastic importance function from an algorithm known as a weight-window generator. We call the tetrahedral-mesh version of this automatic variance-reduction package AVATAR-TET. To demonstrate the effectiveness of AVATAR-TET we consider two problems: an iron "brick" problem, and a slight variation on the nuclear oil-well logging tool problem previously considered.

The geometry of the "brick" problem consists of an iron brick with dimensions 10 cm x 10 cm x 10 cm. An isotropic point source is placed at (0.25,4.25,2.25) cm and a scalar flux tally is scored in a small cell centered at (9.75,9.75,9.75) cm. Four calculations were performed for this problem. Each calculation was performed using one of the following four variance-reduction techniques: analog (no variance reduction), AVATAR, AVATAR-TET, and the MCNP weight-window generator. The results are summarized in Table 2. The data in the table is to be interpreted as follows. "Mean" refers to the mean estimate for the flux talley. "Error" refers to the one-sigma standard relative deviation in the mean talley estimate. "FOM" refers to the "figure of merit", which is proportional to the efficiency of the calculation. Specifically, the FOM is equal to the inverse of the product of the Monte Carlo run time in minutes and the square of the one-sigma standard relative deviation.

Table 2. Results for the iron brick problem.

Variance Reduction	Mean	Error	FOM
analog	3.7040	0.0433	8.7
AVATAR	3.2403	0.0453	20
AVATAR-TET	3.1309	0.0741	27
MCNP generator	3.4969	0.0512	20

The data given in Table 2 indicate that AVATAR-TET is about 40 percent more efficient than the other variance-reduction schemes, and about three times more efficient than the analog calculation.

Each of the four problems was run until all ten of the MCNP statistical tests were passed. Passing these tests indicates that the error estimate is statistically valid. A valid error estimate is required to compute a reliable FOM. The total computer time (Monte Carlo time plus importance-function generation time) required for each calculation is given in Table 3.

Table 3. CPU time breakdown for the brick problem. The importance function generation time includes time required to iterate and/or generate the weight windows. The total CPU time includes the time required to pass all of MCNP's statistical checks.

Problem	Importance function generation (min)	MCNP runtime (min)	Total (min)
AVATAR	1.25	24.08	25.33
AVATAR-TET	~0.5	6.81	7.30
MCNP generator	36.45	19.55	56.0

The data given in Table 3 indicates that the two deterministic adjoints were much cheaper to generate than the stochastic adjoint for this problem. The Monte Carlo run time for AVATAR-TET is about a factor of three smaller than the AVATAR and weight-window generator run times. This might seem to contradict the figure-of-merit data given in Table 2. However, it does not. Longer running times simply imply that more particles had to be run to obtain statistically valid error estimates. Thus the AVATAR-TET calculations were less "noisy" than the other two calculations for this problem. It is not obvious to us why this should be the case. We continue to investigate this question.

The second problem we considered was a slight variation on the neutron--based oil-well logging tool problem described earlier. In particular, the far detector response was tallied rather than the ratio of the near and far detector responses. Three calculations were performed for this problem, each corresponding to one of the three following variance-reduction options: analog, AVATAR and AVATAR-TET. As in the brick problem, both the AVATAR and AVATAR-TET calculations were performed with five energy groups, and each of the three calculations was continued until all 10 of the MCNP statistical tests were passed. The results of these runs are listed in Table 4.

Table 4. Output results for the well-logging problem, far-detector tally.

Problem	Mean	Error	FOM
analog	2.2843E-4	0.0816	1.0
AVATAR	2.0852E-4	0.0236	74
AVATAR-TET	2.1259E-4	0.0280	68

It can be seen from Table 4 that the AVATAR and AVATAR-TET schemes perform comparably for this problem, but AVATAR-TET is a little less efficient than AVATAR. The increase in efficiency relative to the analog calculation is a factor of 74 for the AVATAR scheme and a factor of 68 for the AVATAR-TET scheme. Thus automatic variance reduction is much more effective for the tool problem than the brick problem. Total CPU times for the AVATAR and AVATAR-TET calculations are roughly equivalent. AVATAR-TET would have a slightly larger FOM than AVATAR if it were not for the increased overhead associated with ray tracing through the tetrahedral mesh. It is about 25 percent more costly to ray trace through the tetrahedral mesh than the rectangular mesh associated with AVATAR.

The geometry for the oil-well logging tool problem is fairly complex. We know that the AVATAR-TET importance function is more accurate than the AVATAR importance function. Thus one must ask why AVATAR-TET did not perform significantly better than AVATAR. We believe that the answer lies in the variance reduction technique used in MCNP. There are two basic approaches to variance reduction: biasing and importance sampling. A biasing scheme uses particle splitting to increase the population of "important" particles and Russian roulette to decrease the population of "unimportant" particles.[1,2] An importance sampling scheme replaces the physical interaction probability distributions with modified distributions that effectively ensure that particles contribute to the tally. Biasing schemes are simple to implement and generally have low overhead, while importance

sampling schemes are generally difficult to implement and often have significant overhead.

The automatic variance-reduction scheme used in MCNP is a biasing scheme. A problem with biasing schemes is that they are not nearly as effective as importance sampling schemes when the importance function is rapidly varying. Unfortunately, the most difficult Monte Carlo calculations do in fact have rapidly varying importance functions. We have observed that for very difficult problems, the automatic variance-reduction scheme in MCNP is relatively insensitive to increases in the accuracy of the importance function once a certain level of accuracy has been reached. This is why the performance level is about the same for both AVATAR and AVATAR-TET on the oil-well logging tool problem. To take full advantage of our tertahedral-mesh code for automatic variance-reduction purposes, we believe that we must develop an automatic variance-reduction technique for MCNP that is based upon an importance-sampling technique rather than a biasing technique. This will be the focus of our next research effort.

Publication

Wareing, T. A. , McGhee, J. M. , and Morel, J. E. , "ATTILA: A Three-Dimensional Unstructured Tetrahedral-Mesh Discrete Ordinates Code," *Transactions of the American Nuclear Society,* **75**, 146-147 (1996).

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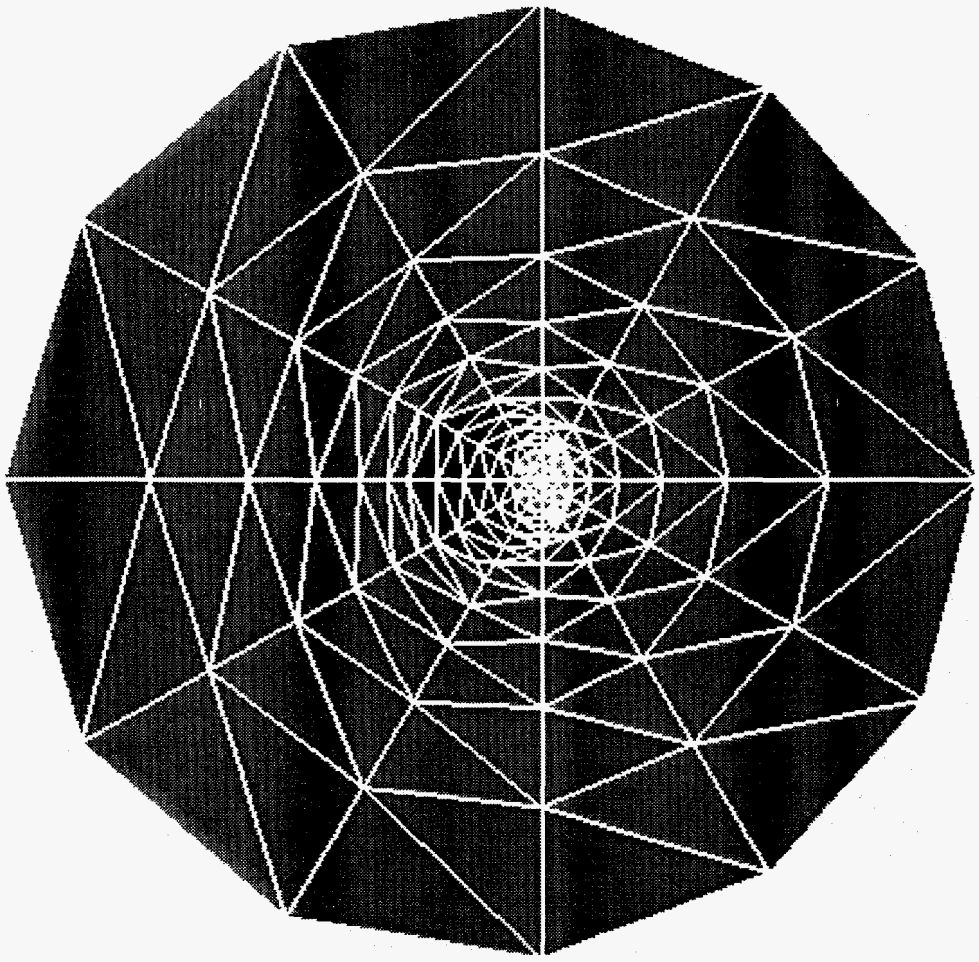

Figure 1. Top view of neutron-based well-logging tool mesh. Shown are the ground, the borehole in the ground, and the tool against the side of the borehole.

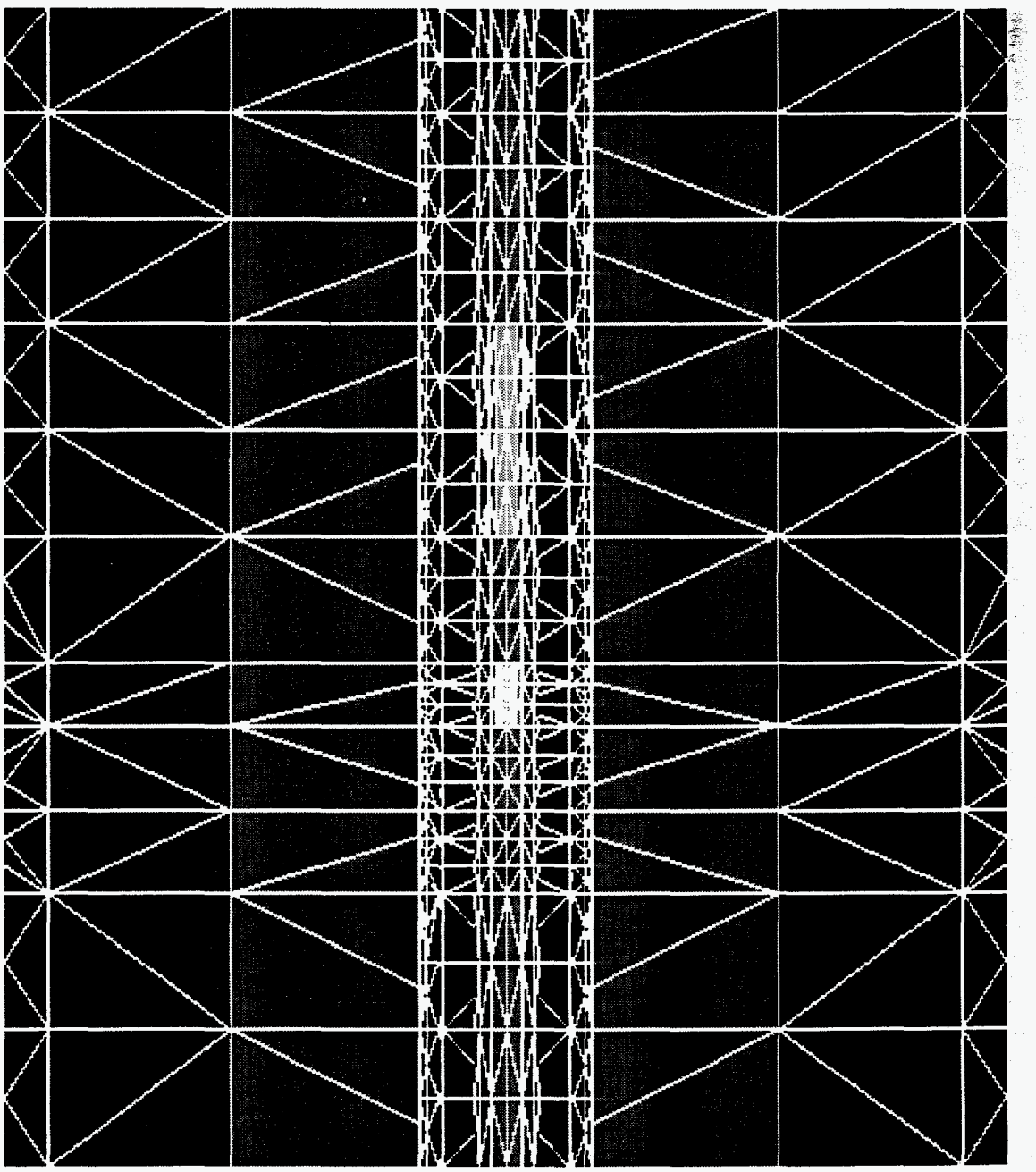

Figure 2. Cut-away side view of neutron-based oil-well logging tool mesh. Note that only a small portion of the mesh is shown.