

3-D DETERMINISTIC TRANSPORT METHODS RESEARCH AT LANL UNDER ASCI

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ABSTRACT

The 3-D deterministic transport methods research that has been done at Los Alamos National Laboratory under the auspices of the ASCI program is briefly described, and future research directions are discussed. The research that has been done relates to the development of both numerical methods and parallel solution algorithms. Such methods and algorithms have been developed for the standard first-order form of the transport equation, second-order self-adjoint forms of the transport equation, S_n and P_n angular discretizations, and 3-D structured and unstructured meshes. New 3-D unstructured-mesh methods make it possible to efficiently apply the S_n method to problems with complex 3-D geometries. New parallel solution algorithms make it possible to perform calculations that are far beyond the capabilities of the best vector supercomputers. Nonetheless, there is much room for improvement in both numerical methods and parallel algorithms. The development of efficient parallel algorithms for the standard first-order S_n equations on unstructured meshes is a significant challenge, but the potential benefits of such methods are enormous.

1. INTRODUCTION

The purpose of this paper is to describe the 3-D deterministic transport methods research that has been done at Los Alamos National Laboratory (LANL) under the auspices of the Accelerated Strategic Computing Initiative (ASCI) program. In accordance with ASCI priorities, the Transport Methods Group at LANL (Group X-6) has significant research efforts in three-dimensional methods for neutron and thermal radiation transport calculations. All ASCI transport methods development done at LANL falls under one of the following two categories:

- development of *numerical methods* for discretizing the transport equation and solving the discretized equations;
- development of *parallel solution algorithms* for applying numerical solution techniques in a parallel manner.

The ASCI research activities in the Transport Methods Group are organized into the following thrust areas:

- parallel algorithms for the standard first-order form of the transport equation on rectangular meshes;
- numerical methods and parallel algorithms methods for second-order self-adjoint forms of the transport operator on unstructured meshes;
- numerical methods and parallel algorithms for the standard first-order form of the transport equation on unstructured meshes.

In the remainder of this paper, our accomplishments in each of the thrust areas are first discussed, followed by a discussion of current research activities.

2. RECTANGULAR-MESH ALGORITHMS

Our first efforts in the development of parallel algorithms for rectangular meshes focused upon techniques for performing a 3-D S_n sweep¹ in parallel. The algorithm that was developed (which we refer to as the KBA algorithm²) exploits the inherent parallelism associated with a planar sweep in 3-D. A 1-D sweep is inherently sequential. For instance, for any given direction on a 1-D mesh with N cells, N “steps” are required to complete the sweep with the outgoing fluxes calculated for a single cell at each step. However, in multidimensional sweeps, one can solve for outgoing fluxes in several cells at each step. For instance, on a 2-D rectangular $N \times N$ mesh, $2N-1$ steps are required to complete the sweep, and the outgoing fluxes calculated for N cells (on the average) in each step. On a 3-D rectangular $N \times N \times N$ mesh, $3N-2$ steps are required to complete the sweep, and the outgoing fluxes calculated for N^2 cells (on the average) in each step. Thus the inherent parallelism in a 3-D sweep is quite high. The transport community did not generally appreciate this until the KBA algorithm was published. In fact, the S_n sweep algorithm was often put forth in the parallel computing community as an example of an inherently sequential algorithm. The latest parallel sweep algorithm for rectangular meshes is implemented in the LANL S_n code, PARTISN, which is a follow-on to DANTSYS/MPI³. This code gives excellent parallel performance on the ASCI-RED machine at Sandia National Laboratories (SNLA)⁴. In particular, parallel efficiency on the order of 80 percent is achieved in a “weak” scaling study with 3000 processors. In a weak scaling study, the problem size is increased as the number of processors was increased so that the number of unknowns per processor remains fixed. With a perfectly parallel solution algorithm, the time-to-solution remains constant as the number of processors is increased. We define the parallel efficiency as the time-to-solution (wall clock) with one processor divided by the time-to-solution with N processors. Thus with an efficiency of 80 percent, PARTISN took 25 percent longer to obtain a solution with 3000 processors than it did with 1 processor. PARTISN also gives excellent parallel performance within a single box on the ASCI-BLUE machine at LANL⁴. Cross-box performance is hampered on the BLUE machine by high latencies associated with cross-box communication. This latency problem is being addressed by using buffering techniques to replace many small messages with a single large message, and by use of the multiple communication ports available within each box. In addition, reduced-latency hardware will eventually be implemented on the ASCI-BLUE machine.

3. SELF-ADJOINT METHODS AND ALGORITHMS FOR UNSTRUCTURED-MESHES

The first unstructured-mesh transport methods developed at LANL were developed for the even-parity transport equation. Our reasons for doing this were as follows:

- Standard continuous finite-element⁵ (CFEM) spatial discretization techniques are easily applied to the even-parity S_n equations on general unstructured meshes, whereas solving the standard S_n equations on such meshes appeared to be highly problematic at the time.
- Solving the even-parity CFEM S_n equations via source iteration requires the solution of many independent diffusion-like sparse symmetric positive-definite (SPD) matrix equations at each iteration step. The computational technology for solving this type of matrix equation is highly advanced both from a numerical methods viewpoint and from a parallel algorithmic viewpoint. Thus efficient numerical methods and parallel solution algorithms originally developed for various diffusion operators were immediately applicable to the solution of the even-parity S_n equations.
- The discretized synthetic acceleration equations consistent with the even-parity CFEM S_n equations take the form of standard CFEM diffusion equations and thus can be solved using the same advanced techniques used for the S_n equations themselves. Synthetic acceleration is much easier to carry out with the even-parity CFEM S_n equations than with the standard S_n equations because the latter generate non-standard discontinuous diffusion discretizations that are difficult to solve. The ability to do fully-consistent synthetic acceleration is essential for thermal radiation transport calculations because the source iteration process generally converges at a prohibitively slow rate.
- Because sparse SPD systems are one of the most common numerical systems arising in science and engineering, many researchers in many disciplines are constantly developing improved methods and algorithms for solving such systems. The even-parity S_n approach enables us to utilize this vast source of research even though it originally may not have been directed towards the transport equation.

In the process of investigating approaches for unstructured-mesh transport calculations, LANL researchers showed that the source iteration process converges for the even-parity S_n equations in the same way that it converges for the standard S_n equations; and that every synthetic acceleration scheme applicable to the standard S_n equations is also applicable to the even-parity S_n equations⁶. This property together with the ease of solving the fully-consistent synthetic acceleration equations made the even-parity S_n equations an overwhelming choice as an initial vehicle for unstructured-mesh thermal radiation transport calculations. As previously stated, the even-parity S_n equations are solved via source iteration. The inner iterations are accelerated via diffusion-synthetic acceleration and the outer iterations are accelerated via the linear multifrequency-grey method. These two schemes are fully described for the first-order form of the S_n equations in reference 7. The multifrequency-grey scheme uses a one-group diffusion operator as the low-order operator and thus is a form of diffusion-synthetic acceleration. These acceleration schemes are extremely effective in terms of the spectral radius of the accelerated source iteration process. However, one must be able to efficiently solve the independent sparse SPD diffusion-like equations associated with the source iteration process and the sparse SPD diffusion equations associated with the acceleration process to achieve an efficient overall solution process. We use the preconditioned

conjugate-gradient method⁸ to solve these equations. At the present time, the preconditioning consists of nothing more than row and column scaling of the matrix. However, much development of advanced parallel preconditioners is occurring under the ASCI program. Algebraic multigrid⁹ is a candidate preconditioner for unstructured meshes. Optimal preconditioners are required to achieve proper weak scaling. An optimal preconditioner is one that gives a condition number that remains bounded as the size of the system increases without bound. At the present time, only multigrid preconditioners are known to be optimal.

The parallel strategy that we use to solve the even-parity equations is quite common and exploits the inherent parallelism present in a matrix-vector product and a vector dot product. The conjugate-gradient method used to solve the source iteration equations is dominated by such products. It is clear that all of the multiplications that occur in a matrix-vector product and a vector dot product can be simultaneously performed. The sums that are required after the multiplications are performed can be carried out in a parallel manner via a reduction algorithm. For instance, suppose that one is given a set of numbers to sum. The reduction algorithm begins by grouping all of these numbers into pairs. Next, all of the pairs are simultaneously summed. At this point, half of the original numbers remain to be summed. The process is then repeated until all of the numbers have been summed. Although this is not a perfectly parallel algorithm, it nonetheless exhibits proper weak scaling. The parallel conjugate-gradient method that we use exhibits proper weak scaling on a per-iteration basis, but not on a time-to-solution basis. This happens simply because the number of conjugate-gradient iterations increases with problem size. As previously mentioned, parallel multigrid preconditioning is needed to achieve the proper weak scaling.

Our latest numerical methods and parallel solution techniques for the even-parity S_n equations are implemented in the LANL code, DANTE¹⁰. DANTE uses a hybrid finite-element mesh (a mesh composed of arbitrary combinations of hexahedra, wedges, pyramids, and tetrahedra, e.g., see Fig. 1). It has options for S_n , P_n , and SP_n angular discretizations and can solve the even-parity, odd-parity, and self-adjoint angular flux (SAAF) forms of the transport equation. The SAAF equation¹¹ offers certain advantages relative to the even-parity and odd-parity equations, but it is not well known within the transport community. It has recently been studied¹¹ by LANL researchers. DANTE gives excellent weak scaling on a per-iteration basis within a single box of the ASCI-BLUE machine at LANL. As is the case for the KBA algorithm, good parallel performance is limited to a single box due to high latency in interbox communications.

4. FIRST-ORDER METHODS AND ALGORITHMS FOR UNSTRUCTURED-MESHES

Many difficulties arise when methods for the standard first-order form of the S_n equation are applied on unstructured meshes. The main source of such difficulties is the slightly curved and reentrant cell faces that commonly occur on general hybrid finite-element meshes. In general, hexahedra, wedges, and pyramids have curved faces, but tetrahedra have flat faces. This is why our initial attempt to develop a 3-D unstructured-mesh method for solving the standard first-order S_n equations focused upon a pure tetrahedral mesh rather than a full hybrid mesh. A linear-discontinuous spatial discretization scheme was applied on tetrahedral meshes, and an algorithm was developed for ordering of the angular flux unknowns associated with a given quadrature

direction so as to achieve a block lower-triangular structure for the sweep equations¹². Each block contains the equations for the flux unknowns associated with a given quadrature direction within a single cell. On 2-D meshes with non-reentrant cells and a non-reentrant mesh, a lower-triangular ordering of the mesh unknowns always exists. We expected this same principle to apply in 3-D, but we eventually discovered that this is not the case. In particular, we found that about one percent of the tetrahedral meshes that we generated did not have a block lower-triangular ordering for one or more directions due to a cyclic dependency between fluxes in different cells. We then developed an algorithm based upon graph theory to “break” each cyclic dependency and arrive at an ordering¹². The dependencies are broken by using incoming flux values from the previous sweep for certain cells in the cycle. Performing the sweep with lagged incoming flux values does not fully solve the sweep equations, but because a very small number of fluxes are lagged, there is no discernable effect upon the convergence of the source iteration process or the effectiveness of convergence acceleration processes. Our latest tetrahedral-mesh methods are implemented in the LANL S_n code, ATTILA¹³. With the addition of a first-collided flux treatment for collimated sources and a last-collided flux treatment for collimated detectors, ATTILA has proven to be a very useful tool for modeling neutron-based and gamma-ray-based oil-well logging tools¹⁴. For instance, when it was used to model a gamma-gamma tool, ATTILA met industrial standards for accuracy while requiring about 10 hours of computing time on a workstation. The same calculation would have required at least several weeks using industry-standard Monte Carlo methods. A tetrahedral mesh for a gamma-gamma logging tool calculation is illustrated in Fig. 2.

After developing tetrahedral-mesh methods, we developed a standard first-order S_n method for general hybrid finite-element meshes (see Fig. 1 for an example of such a mesh). The slightly curved and reentrant cell faces that are generally encountered on such meshes make the application of discontinuous finite-element (DFEM) methods very difficult because a quadrature direction may be incoming over one portion of a face and outgoing over the remainder of the face. When this occurs, rigorous application of the DFEM method requires an additional discontinuity in the solution that makes certain integrals that have to be performed over the cell faces extremely difficult to evaluate. Furthermore, if a quadrature direction is both incoming and outgoing on a single face, the flux unknowns for that direction will be mutually dependent within the two cells that share that face. Thus a lower-triangular ordering of the flux unknowns for that direction will not exist, and a sweep cannot be performed for that direction. These difficulties were overcome by using an average surface-normal unit vector to uniquely define whether a direction is incoming or outgoing over a curved cell face¹². We stress that this represents an approximation to the rigorous DFEM method for those directions that are both incoming and outgoing on that face. It was next found that cyclic dependencies of the type originally observed on pure tetrahedral meshes often form after this average-normal approximation is made. The origin and nature of these dependencies is not yet fully understood. Nonetheless, when dependencies of any type occur, we use the dependency-breaking algorithm originally implemented in ATTILIA to define an approximate sweep process. While very few cyclic dependencies arise on pure tetrahedral meshes or smooth hexahedral meshes, a significant number routinely arise on well-formed non-smooth hybrid finite-element meshes. We were very surprised to find that these dependencies have no discernable effect upon the accuracy of the scalar flux solution, the convergence of the source iteration process, or the effectiveness of convergence acceleration processes. It appears that this insensitivity can be attributed to the fact that cyclic dependencies are caused by directions that are nearly parallel to a cell face. With DFEM discretizations, an incoming flux that is exactly parallel

to a flat cell face makes no contribution to the flux solution within the cell. Thus we speculate that incoming fluxes nearly parallel to a slightly curved cell face make a relatively small contribution to the flux solution within the cell associated with that face. This is apparently why lagging such incoming flux values in a sweep has a negligible effect on the accuracy of the flux solution and the efficiency of the solution process itself. Our unstructured-mesh methods for the standard first-order S_n equations are described in detail in reference 12. Our latest methods for solving the standard first-order S_n equations on 3-D unstructured hybrid finite-element meshes are implemented in a LANL code called PERICLES. Our experience with PERICLES is not nearly as extensive as our experience with ATTILA. One of the main reasons for this is that commercial tetrahedral-mesh generators are currently far more capable of modeling extremely complex geometries than hybrid finite-element mesh generators. However, the hybrid mesh-generation technology is constantly improving and may ultimately prove superior to the tetrahedral-mesh technology.

Research on parallel algorithms for unstructured-mesh sweeps is ongoing at LANL. This is a very difficult problem. The domain decomposition required for proper weak scaling is extremely difficult to achieve for a general unstructured mesh. Far more research is required to fully understand this problem. Thus we do not currently have a parallel capability for solving the standard first-order S_n equations on 3-D unstructured meshes.

5. CURRENT RESEARCH DIRECTIONS

The following research topics are either currently being investigated at LANL or will be investigated in the near future:

2. optimal preconditioners for DSA equations fully consistent with DFEM S_n spatial discretizations on 2-D and 3-D unstructured meshes;
3. block adaptive spatial mesh refinement techniques and associated parallel solution algorithms for the S_n equations, with application to neutronics;
4. cell-by-cell adaptive spatial mesh refinement techniques and associated parallel solution algorithms for the S_n equations and the variable Eddington tensor equations, with application to thermal radiation transport;
5. cell-centered self-adjoint S_n and P_n spatial discretizations using mixed hybrid finite-element methods and support-operators methods;
6. spatial discretizations for the S_n equations on 2-D and 3-D unstructured meshes; with application to thermal radiation transport;
7. parallel S_n sweep algorithms on unstructured meshes;
8. ray-effect mitigation;
9. discretization and fully implicit non-linear solution techniques for the radiation-hydrodynamics equations with strong coupling between the hydrodynamics and radiation fields.

CONCLUSIONS

Funding from the ASCI program is enabling LANL to engage in a wide spectrum of transport methods and parallel algorithms research. Our capabilities for performing deterministic 3-D radiation transport calculations with complex geometries have dramatically improved over the last several years and continue to improve. Our ability to utilize new and powerful parallel computers also continues to improve, but full utilization of commercial massively-parallel systems has yet to be achieved. Nonetheless, we can now do practical engineering calculations on parallel supercomputers that are impossible to do using the most powerful vector supercomputers.

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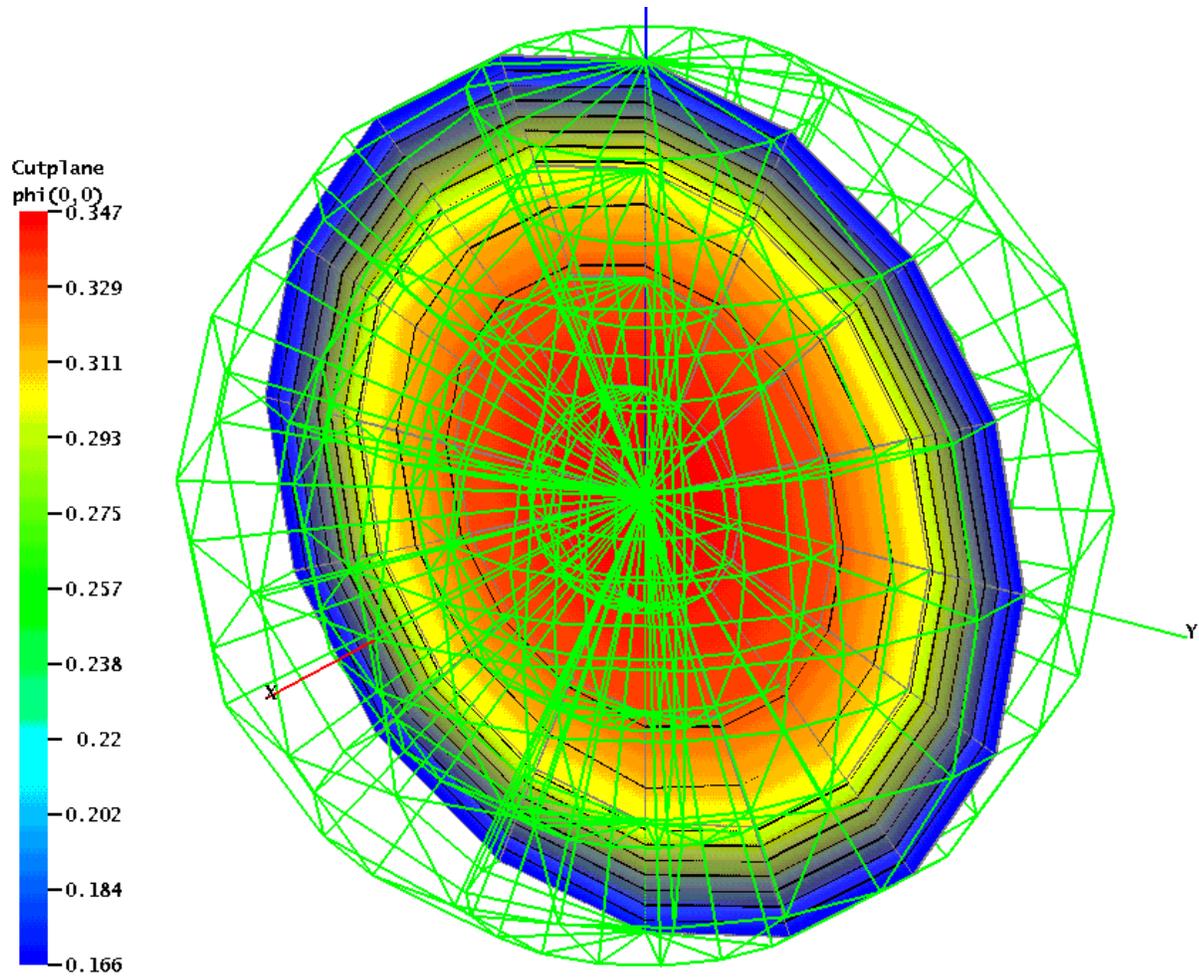


Figure 1. Example of a Hybrid Finite-Element Mesh with Solution Contours on a Cut-Plane. This spherical mesh has pyramids at the center, wedges at the poles, and hexahedra everywhere else. An S_n calculation was performed with the PERICLES code using this grid. The scalar flux color contours are shown on a plane cutting through the center of the sphere. Red corresponds to high scalar flux values and blue corresponds to low scalar flux values.

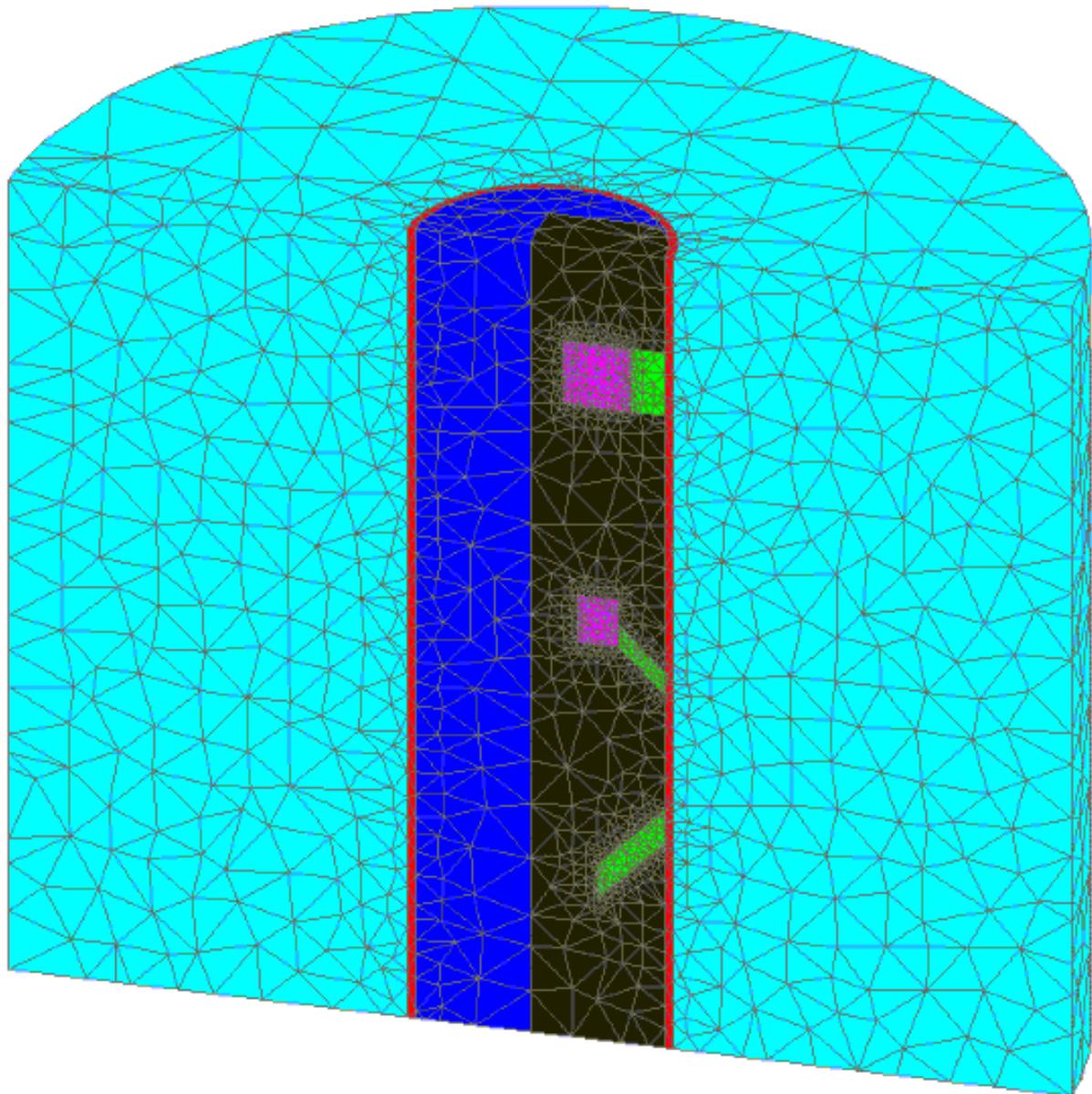


Figure 2. Example of a Tetrahedral Mesh for Modeling a Gamma-Gamma Oil-Well Logging Tool. Shown is the rock strata (turquoise), a thin mudcake layer about the borehole (red), the borehole (blue), the tool (black), a collimated radiation source (green), and two collimated detectors (green and violet).