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Transport Methods**

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Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). We have developed a method for solving the neutral-particle transport equation on 3-D unstructured hexahedral meshes using a S_n discretization in angle in conjunction with a discontinuous finite-element discretization in space and a multigroup discretization in energy. Previous methods for solving this equation in 3-D have been limited to rectangular meshes. The unstructured-mesh method that we have developed is far more efficient for solving problems with complex 3-D geometric features than rectangular-mesh methods. In spite of having to make several compromises in our spatial discretization technique and our iterative solution technique, our method has been found to be both accurate and efficient for a broad class of problems.

Background and Research Objectives

The purpose of this work is to develop a discrete-ordinates or S_n method [1] for solving the neutral-particle transport equation on 3-D hybrid finite-element meshes. Such meshes consist of arbitrary combinations of hexahedra and degenerate hexahedra, i.e., wedges, pyramids, and tetrahedra. Traditional methods for solving the 3-D transport equation have been limited to rectangular meshes. Unstructured meshes are far more efficient for modeling complex 3-D objects than rectangular meshes. However, fundamental difficulties are encountered when applying traditional numerical discretization and solution techniques for the transport equation on unstructured hybrid finite-element meshes. The primary objective of our research was to overcome these difficulties without suffering a significant loss of accuracy or efficiency. We later demonstrate that this objective was accomplished.

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

Neutral-particle transport is of fundamental importance to a wide range of LANL and DOE programs. For instance, neutron transport plays a fundamental role in nuclear reactor design and analysis, criticality safety, and health physics. Thermal radiation transport plays a fundamental role in astrophysics, inertial-confinement fusion, and combustion.

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Therefore improvements in neutral-particle transport methods impact a broad spectrum of LANL and DOE programs. The research described in this report has already brought tangible benefits to the ASCI (Accelerated Strategic Computing Initiative) Program.

Scientific Approach and Accomplishments

The fundamental unknown in the transport equation is the angular flux. The angular flux is closely related to the phase-space number density, and is a function of time, space, direction, and energy. The transport equation must be discretized before it can be solved numerically. This is usually done using either a finite-difference or finite-element discretization in time and space, the S_n discretization in direction, and the multigroup discretization in energy. We use the term " S_n equations" to refer to the transport equation with S_n angular discretization and multigroup energy discretization.

The S_n equations are iteratively solved using the source iteration technique. This is a simple matrix splitting technique that iterates on source terms that are coupled in angle and energy. Each source iteration requires the solution of a separate time- and space-dependent equation for each discrete angle and energy. On rectangular meshes, each of these equations can always be placed in a block lower-triangular form by properly ordering the discrete flux unknowns. Each block consists of the unknown fluxes for a given direction and energy within a spatial cell. This block lower-triangular form enables the source iteration equations to be rapidly solved using a direct solution technique for each block in conjunction with back-substitution. Because the solution process moves across the mesh in a manner defined by the ordering of the unknowns, the solution process is often referred to as a "sweep".

Applying discontinuous finite-element spatial discretization techniques to the S_n equations is straightforward on rectangular meshes. There is an independent polynomial representation for the angular flux solution within each spatial cell. Thus the solution is continuous on the interior of each cell. However, since two cells share each face on the interior of the mesh, the solution on each interior-mesh face would appear to be doubly defined. This is remedied by declaring the angular flux on each face to be defined by the solution within the cell from which the radiation emerges. Thus the flux solution on each face is placed upwind relative to the direction of flow of the radiation. Since the cell faces on a rectangular mesh are flat, all of the radiation associated with a given direction emerges from only one of the two cells sharing each interior-mesh face. Thus the solution is continuous on the surface of each face,

but will discontinuously jump as one moves off the face into the cell that the radiation is flowing into. Since the finite-element solution is continuous on the surface of each face and within the volume of each cell, standard numerical quadrature formulae can be used to efficiently and accurately perform the integrals over the cell faces and the cell volumes that contribute to the finite-element matrix coefficients.

On hybrid finite-element meshes, cell faces are generally not flat. If a given direction is incident on one part of an interior-mesh cell face and emergent on another part of the same face, the angular flux solution will be discontinuous at the boundary between the incident and emergent portions of the face. This discontinuity makes it very difficult to perform the surface integrals needed to obtain the finite-element coefficients. Standard quadrature formulae will generally be quite inaccurate for a discontinuous integrand. Furthermore, the equations for the angular flux in a direction that is both incident and emergent from the same face will be coupled within the two cells sharing that face. We refer to such coupling as a two-cell dependency. The presence of such a dependency means the source iteration equations for that direction do not have a block lower-triangular form and cannot be solved via a sweep. In addition, we found that two-cell dependencies are not the only mechanism for losing a block lower-triangular form for the source iteration equations on hybrid finite-element meshes. Cyclic dependencies can arise among any number of cells if the mesh is non-orthogonal. This can occur even if all of the cell faces are flat. We refer to such dependencies as a ring because the cells that give rise to the dependency form a physical structure reminiscent of a ring.

Thus we see that two major problems can arise on hybrid finite-element meshes that do not arise on rectangular meshes. Specifically, discontinuities can arise on cell faces rendering standard quadrature formulae inexact, and the lower block-triangular form of the source iteration equations can be lost due to either two-cell dependencies caused by these discontinuities or dependency rings arising for geometric reasons.

Our strategies for circumventing these difficulties are based upon three observations. The first is that all of these difficulties arise from flux in directions that are nearly parallel to a face. Second, in the limit as the direction of flux incident upon a flat cell face becomes parallel to that face, the solution within the cell into which the flux is flowing approaches zero. Thus nearly parallel or "grazing incidence" fluxes have a weak effect upon the solution. Third, the probability of having a flux both incident and reflecting on the same cell face is proportional to the curvature of the face. A high degree of curvature is indicative of an inaccurate mesh. Therefore difficulties with grazing-incidence fluxes should rarely arise on "good" meshes.

We circumvent these difficulties using the following procedures. First, directions are declared to be either incident or exiting on an entire face using an average normal vector for the face. This sets the upwind direction for the solution.

This eliminates any discontinuity in the solution on the cell face and allows standard quadrature formulae to be used for the finite-element surface integrals. However, it is important to recognize that an approximation to the standard finite-element technique is being made, so a significant degradation in accuracy would appear possible. Elimination of the discontinuities on the cell faces also eliminates the two-cell dependencies, but the lower-triangular form of the source iteration equations can still be lost through the formation of dependency rings. To deal with dependency rings, we first use graph theory to identify them. Then each dependency ring is "broken" by assuming that one of the angular flux unknowns associated with that ring is known, i.e., by using a value for that unknown from the previous source iteration. This enables us to proceed with an ordering of the flux unknowns and thereby define a sweep. This represents an approximation to the standard sweep process because it no longer yields an exact solution to the source iteration equations.

The approximations that we make to the standard finite-element method and the standard source iteration process could conceivably reduce the accuracy of the finite-element approximation and degrade the efficiency of the source iteration process. To estimate the significance of such effects, we performed a large series of computational tests. Two types of meshes were used in these tests. The first type is a smooth mesh composed of hexahedra. This grid was generated with a commercial grid generation program and approximates a sphere. The cells in this mesh are only slightly skewed. The second type is a non-smooth randomized mesh composed of hexahedra. This type of mesh is obtained by randomly perturbing the vertices of a uniform cubic rectangular mesh. The vertices on the surface of the cube are perturbed but constrained to remain on the surface of the cube. The maximum displacement of any vertex is 15 percent of the width of an unperturbed cell. This results in a mesh that can be considered to be "good" yet still has a significant amount of cell-face curvature.

The main results of our computational tests can be summarized as follows. On a smooth spherical mesh, the number of two-cell dependencies observed corresponds to about 0.2 percent of the maximum number possible. On a non-smooth cubic random mesh, the number of two-cell dependencies observed corresponds to about 4 percent of the maximum possible number. Thus, as would be expected, more two-cell dependencies are observed on non-smooth meshes than on smooth meshes.

The spatial rate of convergence of the scalar (angle-integrated) flux solution on non-smooth cubic random meshes is third order. This would indicate no significant degradation in accuracy since this is the expected convergence rate for the standard (unmodified) finite-element method. Finally, no degradation of the source iteration process was detected on either mesh.

Additional testing was performed beyond that described here. Our overall conclusion is that our transport method for hybrid hexahedral meshes is both accurate and efficient as long as "good" meshes are used. Thus we conclude that our hybrid unstructured-mesh S_n method represents a powerful new capability for neutral-particle transport calculations.

In conclusion we note that we also developed a technique for accelerating the convergence of the source iterations in time-dependent calculations. In addition, we added a charged-particle capability to our method by including the continuous-slowing-down operator in the transport equation and discretizing that operator using a discontinuous finite-element method in energy. The full details of our neutral-particle work are given in the publications listed below. These papers can be downloaded from the web at <http://www-xdiv.lanl.gov/XTM/>.

Publications

1. Wareing, T. A., McGhee, J. M., Morel, J. E., and Pautz, S. D., "Discontinuous Finite-Element S_n Methods on 3-D Unstructured Grids," Proceedings of the International Conference on Mathematics and Computation, Reactor Physics and Environmental Analyses in Nuclear Applications, Madrid, Spain, September 27-30, 1999, Vol. 1, pp.251-261 (1999). An extended version of this paper has been submitted to Nuclear Science and Engineering.
2. Wareing, T. A., Morel, J. E., and McGhee, J. M., "A Diffusion-Synthetic Acceleration Method for the S_n Equations with Discontinuous Finite-Element Space and Time Differencing," Proceedings of the International Conference on Mathematics and Computation, Reactor Physics and Environmental Analyses in Nuclear Applications, Madrid, Spain, September 27-30, 1999, Vol. 1, pp.45-54 (1999). An extended version of this paper will be submitted to Nuclear Science and Engineering.

References

- [1] Lewis, E. E. and Miller, W. F., Computational Methods of Neutron Transport, American Nuclear Society, Inc., La Grange Park, Illinois (1993).