LA-UR- 98-1373

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Title: A FIRST COLLISON SOURCE MEETING FOR ATTILA, AN UNSTRUCTURED TETRAHEDRAL MESH DISCRETE ORDINATES CODE

CONF-980403--

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Submitted to: TOPICAL MEETING ON RADIATION PROTECTION AND SHIELDING, APRIL 19-23, 1998, NASHVILLE, TN

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A First Collision Source Method For ATTILA, An Unstructured Tetrahedral Mesh Discrete Ordinates Code

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Abstract

A semi-analytic first collision source method is developed for the transport code, ATTILA, a three-dimensional, unstructured tetrahedral mesh, discrete-ordinates code. This first collision source method is intended to mitigate ray effects due to point sources. The method is third-order accurate, which is the same order of accuracy as the linear-discontinuous spatial differencing scheme used in ATTILA. Numerical results are provided to demonstrate the accuracy and efficiency of the first collision source method.

1. INTRODUCTION

We have recently developed a new code, ATTILA[1], a three-dimensional, discrete-ordinates (S_n) code. The main innovation of ATTILA is the fact that it solves the discrete-ordinate equations on an unstructured tetrahedral mesh. This type of mesh allows for accurate modeling of geometrically complex problems. ATTILA employs the linear discontinuous (LD) finite-element spatial differencing scheme. The LD scheme approximates the angular flux within each tetrahedron as a linear function, resulting in four unknowns per tetrahedron. The angular flux is allowed to be discontinuous at the boundaries. The four unknowns are located at the corners (nodes). The scattering source is also represented by four discrete values at the corners of each tetrahedron. The LD scheme allows for relatively coarse meshes as opposed to the traditional diamond or weighted diamond differencing scheme used in many existing production transport codes. As with most discrete-ordinates codes, ATTILA uses the multigroup method for the energy discretization. Diffusion synthetic acceleration is used to accelerate the within-group scattering iterations.

As with any discrete-ordinates code, ray-effects are an inherent problem, especially for shielding type problems with optically thin regions and localized (point) sources. Although ray-effects may be mitigated by increasing the quadrature order, this is often computationally prohibitive. To mitigate ray-effects, many discrete-ordinates codes employ first collision source methods[2]. Such methods are characterized by a decompostion of the flux into its uncollided and collided components. The uncollided flux is calculated analytically and the collided flux is calculated with the discrete-ordinates method. To date such first collision source methods have been limited to rectangular meshes. In this paper we describe a semi-analytic first collision source method for use on unstructured tetrahedral meshes. At the present time, the method is for isotropic point sources only. The method is third-order accurate, consistent with that of the LD spatial differencing scheme in ATTILA. The method preserves global balance (conservation), but does not preserve balance on a cell-by-cell basis.

The remainder of this paper is as follows: in Section 2; we describe the theory of the first collision source method; in Section 3, we provide numerical results to demonstrate the accuracy and efficiency of the first collision source method; and in Section 4, we draw some conclusions.

2. THEORY

Although our method is developed for multigroup problems, each group is done seperately and we only need to consider one group at a time. Let us consider the standard one-group transport problem with vacuum boundaries and an isotropic point source at $\mathbf{r}_\mathrm{p}$:

$$\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},\mathbf{\Omega})+\sigma_t(\mathbf{r})\psi(\mathbf{r},\mathbf{\Omega})=\sum_{l=0}^{L}\frac{2l+1}{4\pi}\sigma_s^l(\mathbf{r})\sum_{m=-l}^{l}Y_{l,m}(\mathbf{\Omega})\Phi_l^m(\mathbf{r})+\frac{q_p}{4\pi}\delta(\mathbf{r}-\mathbf{r}_\mathrm{p}) \ , \tag{1}$$

where the spherical harmonics moments of the angular flux are defined by

$$\Phi_l^m(\mathbf{r})=\int d\mathbf{\Omega}Y_{l,m}(\mathbf{\Omega})\psi(\mathbf{r},\mathbf{\Omega}) \ . \tag{2}$$

Here,

$$Y_{l,m}=\begin{cases}C_l^m P_l^{|m|}(\mu)\cos(|m|\phi) & m\geq 0\\ C_l^m P_l^{|m|}(\mu)\sin(|m|\phi) & m<0\end{cases} \ , \tag{3}$$

$$C_l^m=\sqrt{(2-\delta_{m,0})\frac{(l-|m|)!}{(l+|m|)!}} \ . \tag{4}$$

Here, $P_l^m(\mu)$ are the associated Legendre polynomials. Now let us define,

$$\psi(\mathbf{r},\mathbf{\Omega})=\psi^{(u)}(\mathbf{r},\mathbf{\Omega})+\psi^{(c)}(\mathbf{r},\mathbf{\Omega}) \ , \tag{5}$$

where $\psi^{(\mathrm{u})}$ is the uncollided angular flux and $\psi^{(\mathrm{c})}$ is the collided flux. Problem (1) can be described by the following two equations:

$$\mathbf{\Omega}\cdot\nabla\psi^{(u)}(\mathbf{r},\mathbf{\Omega})+\sigma_t(\mathbf{r})\psi^{(u)}(\mathbf{r},\mathbf{\Omega})=\frac{q_p}{4\pi}\delta(\mathbf{r}-\mathbf{r}_\mathrm{p}) \ , \tag{6}$$

$$\mathbf{\Omega}\cdot\nabla\psi^{(c)}(\mathbf{r},\mathbf{\Omega})+\sigma_t(\mathbf{r})\psi^{(c)}(\mathbf{r},\mathbf{\Omega})=\sum_{l=0}^{L}\frac{2l+1}{4\pi}\sigma_s^l(\mathbf{r})\sum_{m=-l}^{l}Y_{l,m}(\mathbf{\Omega})\Phi_l^{m,(c)}(\mathbf{r})+q_s^{(u)}(\mathbf{r}) \ , \tag{7}$$

where the first collision source, $q_s^{(u)}$, is defined as

$$q_s^{(u)}=\sum_{l=0}^{L}\frac{2l+1}{4\pi}\sigma_s^l(\mathbf{r})\sum_{m=-l}^{l}Y_{l,m}(\mathbf{\Omega})\Phi_l^{m,(u)}(\mathbf{r}) \ . \tag{8}$$

Equation(6) can be solved analytically for the uncollided angular flux:

$$\psi(\mathbf{r})=\delta(\mathbf{\Omega}-\mathbf{\Omega}_r)\frac{\mathrm{q_p}}{4\pi}\frac{e^{-\tau(\mathbf{r},\mathbf{r}_\mathrm{p})}}{|r-r_p|^2} \ . \tag{9}$$

The spherical harmonic moments of the uncollided angular flux become:

$$\Phi_l^{m,(u)}(\mathbf{r}) = \int d\mathbf{\Omega}\delta(\mathbf{\Omega}-\mathbf{\Omega}_r)Y_{l,m}(\mathbf{\Omega})\frac{q_p}{4\pi}\frac{e^{-\tau(\mathbf{r},\mathbf{r_p})}}{\left|r-r_p\right|^2} = Y_{l,m}(\mathbf{\Omega}_r)\frac{q_p}{4\pi}\frac{e^{-\tau(\mathbf{r},\mathbf{r_p})}}{\left|r-r_p\right|^2} \quad . \tag{10}$$

Here, $\tau(\mathbf{r},\mathbf{r_p})$ is the optical distance between $\mathbf{r}$ and $\mathbf{r_p}$. Eq.(10) is used to generate Eq.(8), which is used as a distributed fixed source in Eq.(7).

The primary component of our first collision source method is to solve Eq.(6) on unstructured tetrahedral meshes. First, for a given tetrahedron in the mesh (see Figure 1), we assign four interior points corresponding to a four-point spatial quadrature integration set. These points are labeled (a-d) in Figure 1. The chosen quadrature set will integrate a linear function over the volume of the tetrahedron exactly and all other functions with third-order accuracy. Using ray-tracing techniques[3] we find the optical distance from the point source to each of the quadrature locations. Eq.(10) is then used to calculate the spherical harmonic moments at each of the four quadrature points. The uncollided spherical harmonic moments are then mapped linearly to the four nodes of the tetrahedron (labeled 1-4 in Figure 1).

At this point, we can use the first collided source generated for each corner of the tetrahedron; however, this does not lead to a conservative method. The uncollided flux balance (conservation) equation is obtained by integrating Eq.(6) over the entire phase space volume (space and angle) of the problem, to obtain:

$$R_T^{(u)} = q_p - R_L^{(u)} \ , \tag{11}$$

where, $R_T^{(u)}$ is the uncollided total reaction rate and $R_L^{(u)}$ is the uncollided leakage rate. We begin by calculating the numerical uncollided leakage rate, $R_L^{(u)}$. This is accomplished by summing up the outgoing leakage rate from each of the triangles on the outer boundaries of the problem. The leakage rate out of each triangle along the boundary is obtained using a 12 point quadrature integration set for the surface integral in conjunction with Eq.(9) for calculating the current at each point. Next we calculate the numerical total reaction rate, $R_T^{(u)}$ as follows:

$$\hat{R}_T^{(u)} = \sum_{k=1}^{N_{tets}}\sigma_{t,k}V_k\frac{1}{4}\sum_{i=1}^{4}\Phi_{0,k,i}^{0,(u)} \ , \tag{12}$$

where N_{tets} is the total number of tetrahedra in the mesh, $\Phi_{0,k,i}^{0,(u)}$ is the uncollided scalar flux at the i-th corner of the k-th tetrahedron and V_k is the volume of the k-th tetrahedron. In general, if we substitute $R_T^{(u)}$ and $R_L^{(u)}$ for $R_T^{(u)}$ and $R_L^{(u)}$, Eq.(11) will not hold. To obtain conservation, we must either keep $R_T^{(u)}$ and modify $R_L^{(u)}$ or keep $R_L^{(u)}$ and modify $R_T^{(u)}$. We choose to keep $R_L^{(u)}$ and modify $R_T^{(u)}$ because the leakage calculation is generally much more accurate than the reaction rate calculation. The reaction rate calculation is particularly prone to error at points near the source. The conservative reaction rate follows from Eq.(11):

$$\hat{R}_T^{(u),new} = q_p - \hat{R}_L^{(u)} \ . \tag{13}$$

We make the numerical reaction rate conservative by calculating a global correction factor, α, such that

$$\hat{R}_T^{(u)}\left(1+\alpha\hat{R}_T^{(u)}\right) = \hat{R}_T^{(u),new} \ . \tag{14}$$

The new spherical harmonic moments are then determined by

$$\Phi_{l,k,i}^{m,(u),new} = \Phi_{l,k,i}^{m,(u)}\left(1+\alpha\sigma_{t,k}\Phi_{0,k,i}^{0,(u)}\right) \ . \tag{15}$$

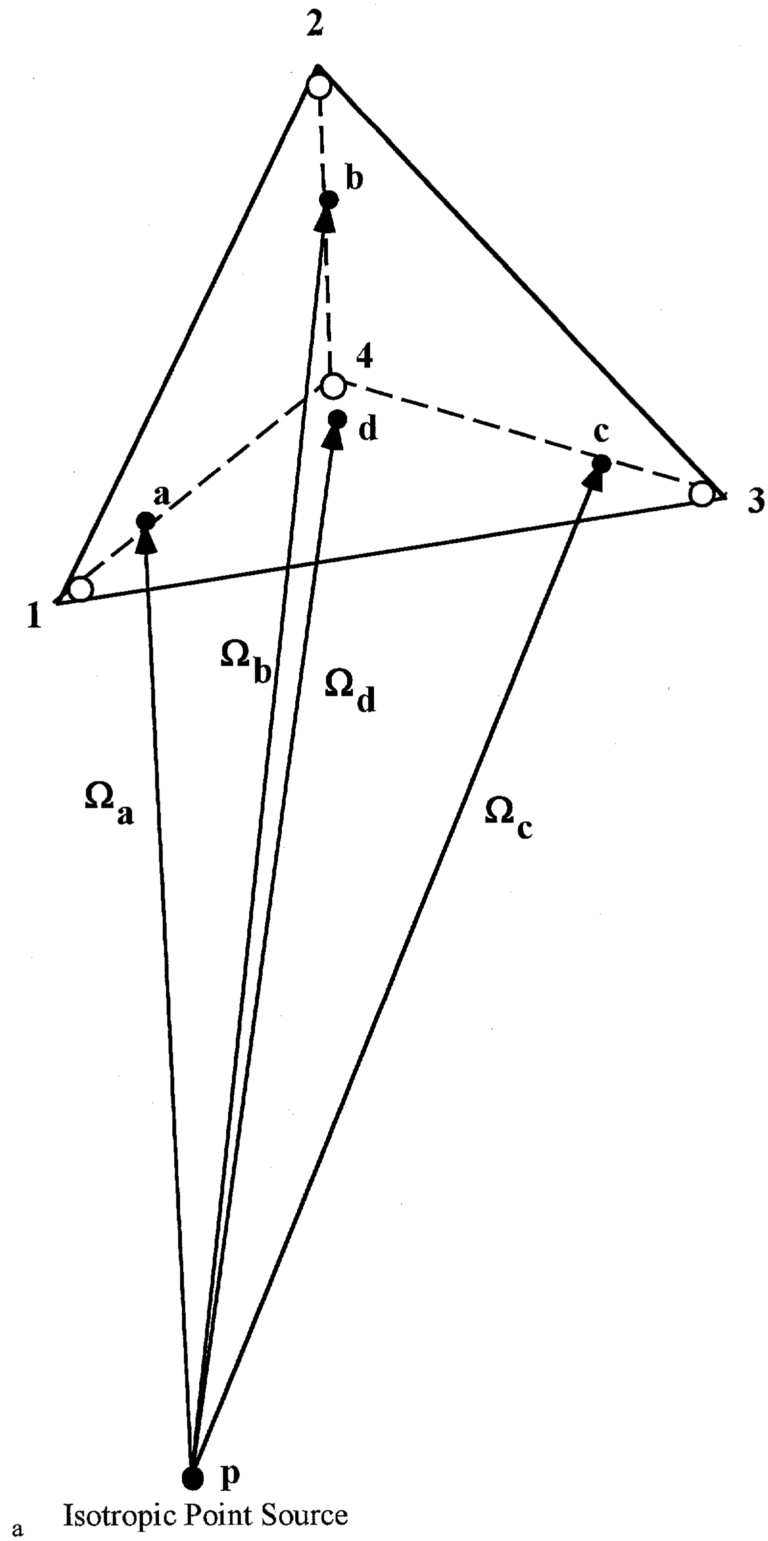

Fig. 1. Diagram of a single tetrahedron including quadrature locations where the uncollided flux is determined.

We note that balance is not maintained on a cell by cell basis.

Finally, we conclude this section by summarizing the method as it applies to ATTILA. After generating the uncollided spherical harmonic moments as described above, we generate the first collision source at each of the four corners of the tetrahedron. We then use ATTILA to solve Eq.(7). The collided spherical harmonic moments from the ATTILA calculation are added to the uncollided spherical harmonic moments to obtain the final solution.

3. NUMERICAL RESULTS

To test the first collision source method in ATTILA, we have developed a simple, yet illustrative problem. The problem consists of a square cube (4cm x 4cm x 4cm) filled with air and centered at x=y=z=0. This cube is centered inside a sphere of iron with a radius of 10 cm. There is a Cf-252 spontaneous fission point source at the origin and a cube detector located in the iron between x=y=z=5 cm and x=y=z=5.5 cm.

The ATTILA model consists of 7481 tetrahedra. We use a 25 group cross section data set with P_3 scattering. As a reference solution, we use multigroup MCNP[4] results using the same 25 group cross sections. All calculations were performed on a SGI R10k Octane workstation. The average energy integrated scalar flux in the detector using multigroup MCNP is $1.126 \times 10^{-3} \pm 0.26\%$ n/(cm^2-s). Table 1 gives the ATTILA detector fluxes and CPU times for varying S_n orders without using the first collision source. Fig. 3 provides a contour plot of the total energy integrated scalar flux along the x-y plane at z=0 without the first collision source and S_6 quadrature. Table 2 gives the ATTILA detector fluxes and CPU times for varying S_n orders using the first collision source. Fig. 2 provides a contour plot of the total energy integrated scalar flux along the x-y plane at z=0 using the first collision source and S_4 quadrature. The results in Tables 1 and 2 clearly show the accuracy and efficiency of the first collision source method. Without the first collision source ray-effects are very pronounced, as can be seen from Fig. 2, and a high S_n order is required to resolve the solution. Using the first collision source, a very low S_n order (even S_4) can resolve the solution, as can be seen from Fig. 3. The timing results show that the first collision source calculation does not significantly increase the overall CPU time for a given S_n order. We note that the slight differences in the ATTILA and MCNP solutions may be attributed to the differences in the anisotropic scattering treatment.

Table 1. ATTILA results without first collision source.

S_n order	Detector energy integrated scalar flux	CPU time (minutes)
4	7.570×10^{-4}	7.88
6	9.260×10^{-4}	13.4
8	1.602×10^{-3}	21.3
12	8.384×10^{-3}	43.3
16	1.136×10^{-3}	75.2

Table 2. ATTILA results with first collision source.

S_n order	Detector energy integrated scalar flux	CPU time (minutes)
4	1.130×10^{-3}	7.50
6	1.126×10^{-3}	14.5
8	1.096×10^{-3}	25.1
12	1.099×10^{-3}	54.6
16	1.101×10^{-3}	99.2

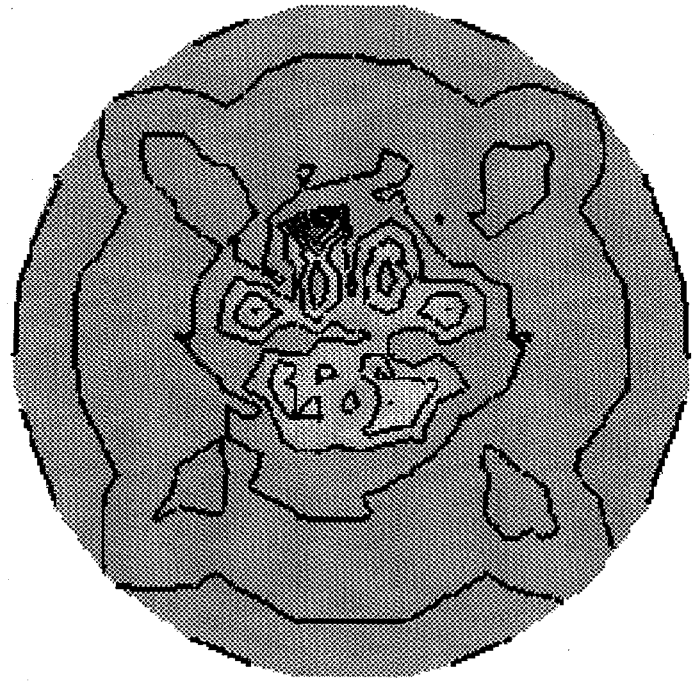

Fig. 2. Isoflux contours along x-y plane at z=0 for sample problem without first collision source using S_6 quadrature.

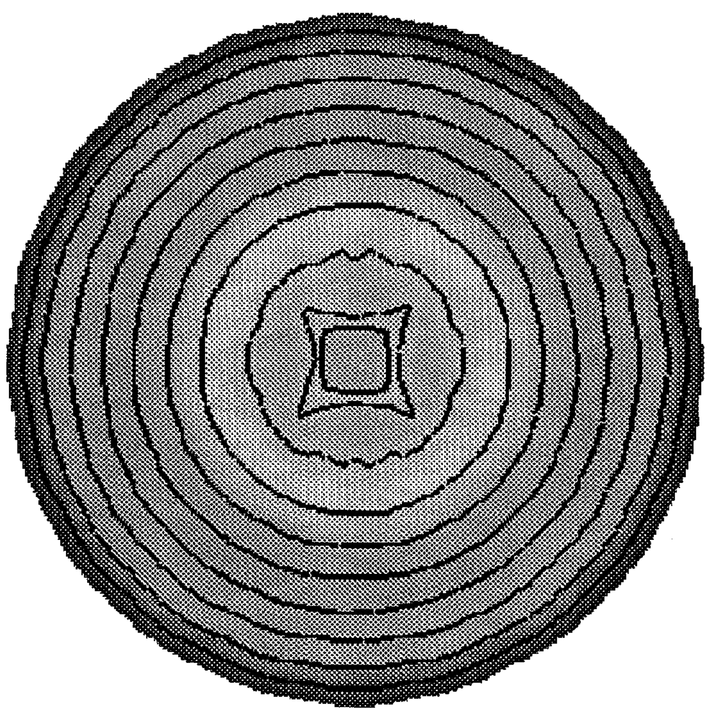

Fig. 3. Isoflux contours along x-y plane at z=0 for sample problem with first collision source using S_4 quadrature.

4. CONCLUSIONS

We have developed a new first collision source method for use on unstructured tetrahedral meshes. The method is implemented into ATTILA, a three-dimensional, unstructured tetrahedral mesh discrete-ordinates code. Numerical results for a simple test problem indicate that the method is accurate and efficient. Future plans include extending this method to unstructured hexahedral meshes.

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