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Use of Discrete Ordinates Methods for Solution of Photon Transport Problems *

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Introduction

Although both neutron and photon distributions are described by the same Boltzmann transport equation, the numerical methods commonly used to solve this equation differ, depending upon which particle distribution is sought. When neutron fluxes are computed, spherical harmonics or discrete ordinates methods are employed, while when photon distributions are calculated, Monte Carlo or moments methods are more frequently used. These latter methods are generally more computationally time consuming than the former, and it is usually held that this is the price paid to adequately represent severely anisotropic photon scattering. That is, most neutron solution codes are capable of representing isotropic and linearly anisotropic scattering; and these approximations, supplemented by the transport approximation, seem to be adequate for many neutron computations. However, in neutron shielding and photon distribution calculations, more precise representation of anisotropic scattering is essential.

Supposing that one wishes to use the same method to compute neutron and photon distributions (in particular, the method of discrete ordinates), the above considerations raise several questions. First, is it even possible, in a multigroup, discrete ordinates representation of the transport equation, to accurately represent severe anisotropic scattering? Even supposing the existence of perfectly prepared multigroup cross sections, might there be some numerical bound on accuracies obtainable? After all, if one is seeking the photon distribution emerging from a reactor-shield complex, one is trying to calculate a distribution that is attenuated by many orders of magnitude; and this distribution must surely be very sensitive to how adequately anisotropic scattering is represented.

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Second, if a discrete ordinates solution is possible, it is economical? That is, must the same amount of computational effort be expended in a discrete ordinates code as in a Monte Carlo code? Third, what sort of scattering approximation should be used? And fourth, how should multigroup cross sections be prepared?

This report describes the results of an investigation undertaken to attempt to answer the above questions. The investigation was restricted to photon transport, primarily because preparation of gamma scattering cross-sections is more amenable to automation. The investigation consisted of four major phases: 1) selection of an anisotropic scattering approximation, 2) modification of a discrete ordinates transport code to apply the scattering approximation, 3) development of a code to produce multigroup photon cross sections for use in the scattering approximation, and 4) testing of the complex constructed in 1), 2) and 3).

The Anisotropic Scattering Approximation

Based on a thorough examination of anisotropic scattering recipes in the monoenergetic Boltzmann equation¹ and the failure of certain extended transport approximations, a $N+1$ term Legendre polynomial expansion was adopted for scattering approximation. Let the collision source term of the Boltzmann equation be written*

$$\iiint \phi(\vec{r}, \vec{\Omega}', E') \sigma_s(E' \rightarrow E, \vec{\Omega}' \cdot \vec{\Omega}) dE' d\Omega' \quad (1)$$

where ϕ is the particle flux as a function of position, direction, and energy, and σ_s is the macroscopic transfer probability for scatter from initial energy E' to energy E through an angle (between initial direction $\vec{\Omega}'$ and final direction $\vec{\Omega}$) with cosine $\mu_0 = \vec{\Omega}' \cdot \vec{\Omega}$. The scattering transfer probability can be expanded in terms of Legendre polynomials of this cosine, giving

$$\sigma_s(E' \rightarrow E, \mu_0) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \sigma_{sn}(E' \rightarrow E) P_n(\mu_0) \quad (2)$$

* σ_s may also be a function of $\vec{r}$. Here, spatial dependence of cross sections is treated by considering a series of homogeneous zones.

where, by orthogonality, the expansion coefficients σ_{sn} are defined by

$$\sigma_{sn}(E' \rightarrow E) = \int_0^{2\pi} \int_{-1}^1 P_n(\mu_0) \sigma_s(E' \rightarrow E, \mu_0) d\mu_0 d\omega \quad (3)$$

In terms of the unit vectors of a spherical coordinate system (for example),

$\vec{e}_r$, $\vec{e}_\theta$, and $\vec{e}_\phi$ and the angles and cosines

$$\mu = \vec{\Omega} \cdot \vec{e}_r$$

$$\eta = \vec{\Omega} \cdot \vec{e}_\theta \equiv \sqrt{1 - \mu^2} \cos \omega \quad (4)$$

$$\xi = \vec{\Omega} \cdot \vec{e}_\phi \equiv \sqrt{1 - \mu^2} \sin \omega$$

the polynomial $P_n(\mu_0)$ can be expanded to give

$$P_n(\mu_0) = P_n(\mu)P_n(\mu') + 2 \sum_{r=1}^n \frac{(n-r)!}{(n+r)!} P_n^r(\mu)P_n^r(\mu') \cos r(\omega - \omega') \quad (5)$$

Here, the P_n^r are associated Legendre polynomials. Similar expansions can be made in other geometries.

The Legendre scattering approximation truncates the expansion of Eq. (2) after the $n = N$ term. The scattering source term of Eq. (1) is then

$$\sum_{n=0}^N \int \sigma_{sn}(E' \rightarrow E) \phi_n(\vec{r}, \vec{\Omega}, E') dE' \quad (6)$$

where

$$\phi_n(\vec{r}, \vec{\Omega}, E') = \frac{2n+1}{4\pi} \iint \phi(\vec{r}, \vec{\Omega}', E') P_n(\mu_0) d\Omega' \quad (7)$$

The Legendre polynomial expansion requires the evaluation of the coefficients, σ_{sn} , of Eq. (3) and of the flux moments, ϕ_n , of Eq. (7). The approximation seems to be accurate with relatively few terms even for exceptionally anisotropic scattering.¹ Qualitatively, both σ_{sn} and ϕ_n should decrease with increasing n . The σ_{sn} are zero, $n > 0$, for isotropic scattering, and fail to decrease with increasing n only in the case of purely forward scattering in which all σ_{sn} are equal. The ϕ_n should decrease because the P_n are (more and more rapidly) oscillating functions while ϕ is positive. Thus, as n increases, the product $\sigma_{sn} \phi_n$ should decrease, and hence become unimportant, rapidly.

In what follows, the truncation of Eq. (6) is referred to as the P_N scattering approximation; and N is the number of terms, in addition to the isotropic term, that are retained. In a discrete ordinates solution of the transport equation the order of angular quadrature, M , is unrelated to N except that, for consistency, M should be greater than N .

Preparation of a Discrete Ordinates Transport Code to Treat Anisotropic Scattering

The DTF² code, a one-dimensional, multigroup, discrete ordinates code, was modified* to accept multigroup transfer cross sections for an arbitrary order, N , of Legendre scattering approximation and to compute the angular moments, ϕ_n . The modified code uses a multigroup analog of Eq. (6) for the source in the g^{th} group, $g = 1, 2, \dots, G$:

$$\sum_{n=0}^N \sum_{h=1}^G \sigma_{sn}^{g \leftarrow h} \phi_{nm}^h \quad (8)$$

Above, ϕ_{nm}^h is the h^{th} group, n^{th} Legendre moment of the angular flux in the discrete direction $\vec{\Omega}_m$:

$$\begin{aligned} \phi_{nm}^h = (2n+1) \sum_{m'=1}^M \omega_{m'} \phi_{m'}^h & \left[P_n(\mu_m) P_n(\mu_{m'}) + \right. \\ & \left. + 2 \sum_{r=1}^n \frac{(n-r)!}{(n+r)!} P_n^r(\mu_m) P_n^r(\mu_{m'}) \cos(\omega_m - \omega_{m'}) \right] \end{aligned} \quad (9)$$

ϕ_{nm}^h is thus a discrete ordinates angular quadrature of the angular flux, $\phi_{m'}^h$, in group h , analogous to the integration of Eq. (7). The factor of 4π is included in the quadrature weight, $\omega_{m'}$. $\sigma_{sn}^{g \leftarrow h}$ is the group h to group g transfer cross section, the analog of $\sigma_{sn}(E' \rightarrow E)$.

The above modification increases code execution time mainly in the time required to prepare and store the moments of Eq. (9). Since the group angular flux

*In addition to the conceptual modification, the code was also re-written in variable dimension Fortran IV to permit more flexible use of storage.

was already available, this increase is surprisingly modest. Execution time is also increased indirectly because an increased order of angular quadrature is needed to accurately integrate the moments of Eq. (9).

Multigroup Cross Sections

Write the general Boltzmann transport equation, with an N term scattering approximation, as

$$\nabla \cdot (\vec{\Omega} \phi) + \sigma_t(E) \phi(\vec{r}, \vec{\Omega}, E) = \sum_{n=0}^N \int \sigma_{sn}(E' \rightarrow E) \phi_n(\vec{r}, \vec{\Omega}, E') dE' + S(\vec{r}, \vec{\Omega}, E) \quad (10)$$

where σ_t is the macroscopic total cross section and S represents external sources.

Let the average flux and external sources in the energy range $E_{g+1} \leq E \leq E_g$ be defined by

$$\begin{aligned} \phi^g(\vec{r}, \vec{\Omega}) &= \int_{E_{g+1}}^{E_g} \phi(\vec{r}, \vec{\Omega}, E) dE \\ S^g(\vec{r}, \vec{\Omega}) &= \int_{E_{g+1}}^{E_g} S(\vec{r}, \vec{\Omega}, E) dE \end{aligned} \quad (11)$$

Then, in terms of the averages

$$\sigma_t^g(\vec{r}, \vec{\Omega}) = \frac{\int_{E_{g+1}}^{E_g} \sigma_t(E) \phi(\vec{r}, \vec{\Omega}, E) dE}{\phi^g(\vec{r}, \vec{\Omega})} \quad (12)$$

and

$$\sigma_{sn}^{g \rightarrow h}(\vec{r}, \vec{\Omega}) = \frac{\int_{E_{h+1}}^{E_h} \phi_n(\vec{r}, \vec{\Omega}, E') dE' \int_{E_{g+1}}^{E_g} \sigma_{sn}(E' \rightarrow E) dE}{\int_{E_{h+1}}^{E_h} \phi_n(\vec{r}, \vec{\Omega}, E') dE'} \quad (13)$$

the group average of Eq. (10) is

$$\nabla \cdot (\vec{\Omega} \phi^g) + \sigma_t^g(\vec{r}, \vec{\Omega}) \phi^g = \sum_{n=0}^N \sum_{h=1}^G \sigma_{sn}^{g \rightarrow h}(\vec{r}, \vec{\Omega}) \phi_n^h(\vec{r}, \vec{\Omega}) + S^g(\vec{r}, \vec{\Omega}) \quad (14)$$

where ϕ_n^h is the denominator of Eq. (13). Equation (14) is a very general multi-group formulation, but the angular flux and its moments are seldom known, even qualitatively.* For the work described here, it is assumed that, at best, only

* Such information can be obtained in an iterative manner. For this purpose the DTF code prints the angular flux moments and their zone averages.

an energy dependent function is available for the averages of Eqs. (12) and (13). Based on this assumption (as a consequence of which σ_t^g and $\sigma_{sn}^{g \leftarrow h}$ are independent of $\vec{r}$ and $\vec{\Omega}$) a code, GAMLEG,³ was written to prepare multigroup photon cross sections. For photon scattering, the Klein-Nishina⁴ differential scattering cross section is given analytically, and the coefficients $\sigma_{sn}(E' \rightarrow E)$ and their E integrals can be obtained explicitly.³ The GAMLEG code is also designed to prepare the group average total cross section as the sum of the scattering cross section average

$$\sigma_s^g = \frac{\int_{E_{g+1}}^{E_g} f(E) dE \int_{E/(1+2E)}^E \sigma_{so}(E \rightarrow E') dE'}{\int_{E_{g+1}}^{E_g} f(E) dE} \quad (15)$$

and the absorption cross section average

$$\sigma_a^g = \frac{\int_{E_{g+1}}^{E_g} f(E) \sigma_a(E) dE}{\int_{E_{g+1}}^{E_g} f(E) dE} \quad (16)$$

Above, $f(E)$ is the energy dependent weighting distribution. The code is designed to accept this weighting function, absorption data, coherent scattering data, and source energy data as input from which the respective group averages are prepared. The energies at which each of these types of data is specified must also be supplied. The energy group structure is chosen by the user. Output is in a form suitable for input to the DTF code.

Test Problems

The test problems here considered are designed as consistency checks, in which the results of one numerical scheme are compared to the results of another, and no effort is made to compare with experiment. In this connection the same raw data (absorption and coherent scattering) was used in each computation. The use made of the data, of course, differed. For example, in the second test problem, the same 81 energy absorption data was used in both solutions. But in the Monte Carlo solution, fluxes were calculated at 81 energies and then condensed for comparison with fluxes, obtained by first group averaging the

absorption data, of the discrete ordinates solution. Similarly, treatment of the collision source differed greatly in the two solutions, but both treatments were based on the Klein-Nishina scattering law.

For lack of better information, the cross sections used in all the discrete ordinates solutions below were prepared with a constant weighting function. An attempt, with unsatisfactory results, to use the source energy distribution as a weighting function is described in Reference 5.

In a first test problem, the percentage of photons penetrating a 10 cm iron slab was computed. A 6 MeV isotropic source was assumed to impinge upon the left side of the slab. The DTF calculation was made using a double P_7 (equivalent to S_{16}) angular quadrature, fifty spatial intervals, and an elementary nine group representation. Unweighted cross section sets were prepared for $N = 0, 1, \dots, 5$. Absorption data was taken from the 81 energy United Nuclear Corporation data file used in conjunction with the Monte Carlo codes, SANE-SAGE⁶ and ADONIS⁷. With unweighted cross sections the only difference between a P_{N-1} and P_N scattering approximation is the addition of the $\sigma_{SN}^{g \leftarrow h}$ scattering transfer matrix. Table I shows the variation of the percentage of the transmitted photons as a function of scattering approximation and group.

Table I. Transmission Percentage - 10 cm Fe Slab^a

Group	Group Energy Bounds (Mev)	P0	P1	P2	P3	P4	P5
1	7.0795-3.5481	2.4574	3.0245	3.10804	3.0553	3.0633	3.0616
2	3.5481-1.7783	0.4979	1.3465	1.4809	1.4285	1.4380	1.4377
3	1.7783-0.89125	0.3703	1.1214	1.2120	1.2032	1.2074	1.2075
4	0.89125-0.44668	0.3424	0.9933	0.9825	0.9953	0.9977	0.9992
5	0.44668-0.22387	0.3854	0.7326	0.6970	0.7064	0.70806	0.7090
6	0.22387-0.11220	0.1671	0.2693	0.2677	0.2699	0.2707	0.2710
7	0.11220-0.05623	0.7127-2	0.9922-2	0.9728-2	0.9810-2	0.9837-2	0.9849-2
8	0.05623-0.02818	0.1916-4	0.2195-4	0.2147-4	0.2163-4	0.2169-4	0.2172-6
9	0.02818-0.01540	0.6433-8	0.6966-8	0.6691-8	0.6715-8	0.6738-8	0.6743-8
Total		4.2277	7.4975	7.7579	7.6685	7.6951	7.6959

^aIn the table $0.7127-2 \equiv 0.007127$.

The above results show a relatively swift convergence pattern. That is, despite the severely anisotropic scattering of 6 MeV photons, the biggest difference between P_3 and P_5 results is 0.64% in the second group. The total P_5 transmission percentage is 2% higher than an ADONIS result. Part of the difference is due to the elementary group structure which does not do justice to the absorption cross section in the lower energy range (cf. the next test problem), and part due to the fact that the ADONIS code does not admit infinite slab geometry.

In a second and more ambitious test, the flux was calculated in a spherical reactor mock-up. The Monte Carlo code SAGE was used to provide comparison results. Since SAGE does not allow a source distributed in energy (except as a superposition of independent monoenergetic problems) a source energy of 2 MeV was arbitrarily chosen. The problem material composition, group structure, and source spatial distribution are given in Table II.

Table II. Reactor Mock-up Specifications

Relative Source Strength	Outer Radius (cm)	Zone	Outer Radius (cm)	Material	Atomic Density ($\times 10^{22}$)	Group Energies (MEV)
1.0	0.97	1	7.74	U-238	1.96	2.00-1.99
0.98	1.94			Fe	1.18	1.99-1.75
0.96	2.91			Na	0.704	1.75-1.50
0.92	3.87	2	9.37	Fe	6.83	1.50-1.25
0.87	4.84			Na	0.395	1.25-1.00
0.81	5.82	3	11.83	Fe	8.3	1.00-0.75
0.74	6.77	4	12.76	Void	---	0.75-0.50
0.65	7.74	5	25.47	Fe	7.5	0.50-0.25
		6	29.52	Fe	4.0	0.25-0.02
		7	80.08	C	6.77	
				B	0.0302	

Initially, a double P_7 angular quadrature, P_5 scattering, and 99 spatial intervals were used in the discrete ordinates solution.

SAGE and DTF fluxes are compared for group 1 in Fig. 1 and for group 7 in Fig. 2. The fluxes are normalized for plotting, but a single normalization factor is used for both sets of data. The agreement of the two solutions in groups

Fig. 1. Group 1 fluxes as a function of radius. $1.99 \leq E_{\gamma} \leq 2.0 \text{ MeV}$.

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Fig. 2. Group 7 fluxes as a function of radius. $0.5 \leq E_\gamma \leq 0.75$ MeV.

2 through 6 is as good as that of group 7. In group 9, however, (Fig. 3) the agreement is not good. The discrepancy here is due to the poor resolution of rapidly varying absorption cross sections in this energy range. To check this statement, a revised group structure was used. The first eight groups were retained intact but group 9 was replaced with groups 9, (0.25-0.20 MeV), 10 (0.20-0.15 MeV), 11 (0.15-0.10 MeV), 12 (0.10-0.05 MeV), and 13 (0.05-0.02 MeV). Both methods were used to recompute fluxes with the comparison as given in Fig. 4 for new group 9, Fig. 5 for group 11 and Fig. 6 for group 13. As shown in the figures, the revised group structure is much more effective than the original.

Since in this problem all the fluxes above 0.05 MeV are attenuated by at least six orders of magnitude in traversing the reactor, the right leakage is sensitive to how accurately the transport equation is solved. Table III shows the effect, on the right leakage, of changing the angular quadrature and refining the spatial mesh.

Table III. Right Leakage by Group (Percent)

Group	99 intervals DP ₇ quadrature	99 intervals P ₁₅ quadrature	148 intervals P ₁₅ quadrature
1	0.001809	0.001909	0.001972
2	0.002153	0.002306	0.002363
3	0.002568	0.002723	0.002787
4	0.002946	0.003107	0.003179
5	0.003572	0.003752	0.003838
6	0.004484	0.004682	0.004786
7	0.005936	0.006144	0.006279
8	0.008919	0.009143	0.009339
9	0.042579	0.043474	0.044249
TOTAL	0.074966	0.077240	0.078791

The Legendre polynomial P₁₅ quadrature is more accurate than the DP₇ quadrature because the former has a direction cosine closer to 1.0. The differences in the right leakages in the problems above are less than that made in more adequately representing the group structure. In the 13 group, 148 interval calculation the total system leakage was 0.0685% compared to the leakage from SAGE of ~0.06% and that of ~0.08% from a run with the Monte Carlo code MCG.⁸

Fig. 3. Group 9 fluxes as a function of radius. $0.02 \leq E_\gamma \leq 0.25$ MeV.

Fig. 4. Revised Group 9 fluxes as a function of radius. $0.20 \leq E_{\gamma} \leq 0.25$ MeV.

Fig. 5. Group II fluxes as a function of radius. $0.10 \leq E_{\gamma} \leq 0.15 \text{ MeV}$.

Fig. 6. Group 13 fluxes as a function of radius. $0.02 \leq E_{\gamma} \leq 0.05 \text{ MeV}$.

For this problem, the discrete ordinate solution required 7.5 minutes (148 interval, 13 group, P_{15} angular quadrature, P_5 scattering) while the Monte Carlo computations each required at least two hours.

A third test calculation was made to examine the effectiveness of the method in problems with energy distributed sources. A uniform source, in radius, was distributed between 0 and 25 cm in a 70 cm iron sphere. The source was distributed in energy as $\exp [-1.1E]$, E in MeV. A detailed definition of the problem and a description of the comparison calculations is given in Reference 5. Figure 7 shows a comparison of group fluxes calculated with the DTF code in two group representations, one chosen to span all energies and the other chosen to refine the high energy behaviour. Figure 8 shows the results of an energy deposition calculation made from DTF fluxes, from methods of moments fluxes, and from Monte Carlo fluxes. A much more detailed comparison of the results is made in Reference 5. The discrete ordinates solution (DP_7 , 24 groups, 99 intervals, and P_3 scattering) required about ten minutes, while the Monte Carlo calculation required over two hours of comparable time. The moments solution required a great deal of "this problem only" computation and no fair time comparison can be made.

Conclusions

As Figs. 1, 2, 4, 5, and 8 show, the discrete ordinates method is able to calculate gamma fluxes in excellent agreement with Monte Carlo and moments solutions. Further, the discrete ordinates method is computationally much faster, at least in one dimensional problems. A portion of this edge might be lost in deep penetration problems where the results of Table III indicate that more care must be taken to calculate emergent fluxes. However, this type of problem is also difficult for Monte Carlo methods since, typically, only a few particles in ten thousand escape.

Fig. 7. Energy dependence of the group fluxes from a exp [-1.1E] source distributed uniformly in the central 25 cm of a 70 cm iron sphere.

Fig. 8. Energy deposition as a function of radius, problem as in Fig. 7.

The test problem results also indicate that the Legendre Scattering approximations are accurate. Except for deep penetration problems when the P_5 or higher approximation is needed, the P_3 approximation seems to be adequate.

The fact that unweighted cross sections give such accurate results seems surprising. However, the results of Fig. 7 show that refining the energy integration mesh in the high energy range did not appreciably alter the flux energy dependence. In the low energy range the distribution altered significantly, but the altered distribution gave the accurate results of Fig. 8. Again, in the second test problem, accuracy in flux computations was achieved when the low energy mesh was refined. From these observations it is concluded that if a fine enough energy mesh is used, unweighted cross sections can give good accuracy. "Fine enough" is, of course, problem dependent, meaning a relatively coarse group structure in the problems considered.

The investigation described above is by no means exhaustive. The test problems form only a small sample, and even in these problems no attempt was made to examine all combinations of quadratures (space, angle, and energy) and scattering approximations (to determine, say, minimum adequate combinations). However, the success, in these test problems, of the combination of multigroup cross sections for a Legendre scattering approximation, discrete ordinates solution of the Boltzmann equation should encourage the use of these methods in other photon transport problems.

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