DISCRETE ORDINATES METHODS FOR RADIATION TRANSPORT

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INTRODUCTION

The discrete ordinates (S_N) method, first developed[1,2] for stellar atmospheres, has been used extensively on various other radiation transport problems. In reactor analysis the method is generally used[3] to generate parameters for design models based on more approximate but less expensive methods (such as diffusion theory) so that the spatial–spectrum coupling is represented accurately on a microscopic reaction rate level. It has a decisive advantage over Monte Carlo methods in computing the pin and assembly power profiles. In shielding problems[4] where the penetration of the radiation can be deep, the method is used widely in design calculations. In oil–well logging problems which also involve deep penetration and have a stringent accuracy requirement on the detector responses, the method complements the Monte Carlo techniques.[5,6] Recently, the discrete ordinates method with appropriate cross sections has been used in coupled photon–electron transport problems.[7]

In this paper we briefly review the basic method, illustrate its applications, discuss its merits and pitfalls, and enumerate the recent advances in the attendant numerical techniques which have enhanced the capabilities of the method.

METHOD

In neutral particle transport of interest in reactor, shielding and well–logging configurations, the time–independent Boltzmann transport equation for the angular flux,

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$\Psi(r,\Omega,E)$, is[8,9]

$$\Omega\bullet\nabla\Psi + \sigma\Psi = S_{ext} + \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(r,E' \rightarrow E,\Omega'\bullet\Omega)\Psi(r,\Omega',E')$$

$$+ \chi(E)\int_0^\infty dE' \int_{4\pi} d\Omega' \nu\sigma_f(r,E')\Psi(r,\Omega',E') \qquad (1)$$

where the phase–space variables, r, Ω, E, Ω', E', and the material properties σ, σ_s, $\nu\sigma_f$ and χ have their usual meanings. In the most commonly used discrete ordinates codes, Eq. (1) is discretized over the phase space variables and solved iteratively to obtain the angular flux and other related quantities.

Phase Space Discretization: Energy is treated by the multigroup and the space variables by the finite difference approximations. The angular variable is represented by a discrete set of directions, Ω_m, the integration over angle replaced by weighted summations, and Eq.(1) is solved for each direction. Recently developed discretization schemes will be discussed later.

Source Iteration: Three levels of iteration can arise for each energy group. These are the inner iteration for within–group scattering, the iteration for those upscattering from lower energy groups and the outer iteration on the multiplication factor due to fission. Since the number of iterations can be very large, techniques[10,11] were devised to accelerate the convergence at each level which result in significant reduction in the computing time.

In conventional finite difference schemes[8,9] the discrete ordinates transport equation in a spatial cell of width Δx, Δy, and Δz is replaced by the difference equation

$$\frac{\mu_m}{\Delta x}(\Psi_R - \Psi_L) + \frac{\eta_m}{\Delta y}(\Psi_F - \Psi_N) + \frac{\xi_m}{\Delta z}(\Psi_T - \Psi_B) + \sigma\overline{\Psi} = \overline{S}\,, \qquad (2)$$

where the subscripts R, L, F, N, T, and B represent the right, left, far, near, top, and bottom surfaces of the cell, and $\overline{\Psi}$ and $\overline{S}$ are the cell–averaged flux and total source, respectively. Auxiliary relations representing the cell–averaged flux as a weighted–average of the cell–surface flux are then used to solve for all the unknowns. The weighting parameters determine the flux shape in the cell. They are set to unity in the step–difference scheme and are $\frac{1}{2}$ in the linear diamond scheme. The latter can yield (unphysical) negative flux for cell widths larger than a mean–free–path and thus requires negative flux fixup schemes. The weighting parameters can also be determined dynamically by requiring the flux to be positive.[10] Given the inflow surface flux from the boundary conditions or from the outflow of the adjacent cells, one marches through the spatial mesh in the direction of particle motion. This iterative process continues until certain specified convergence criteria are satisfied.

The coarse–mesh rebalance (CRB)[10] and the diffusion synthetic acceleration (DSA)[11] schemes are the primary acceleration methods in discrete ordinates codes. In CRB the solution over a coarse mesh (or region) is used to obtain adjustment factors to enforce particle balance after each iteration. In DSA the diffusion equation is solved to provide an extrapolation to the next iteration. Direct[12] and iterative[6] S_2 discrete ordinates solutions has also been used as the initial guess. The major discrete ordinates codes and their salient features will be discussed in the presentation.

EXAMPLE

Figure 1 displays the eigenvalues and power profiles of the benchmark BWR rod bundle problem[13] calculated by two discrete ordinates codes, TWODANT[14] and DORT[15], and the diffusion theory option. The following conclusions can be drawn from these results: 1) The discrete ordinates codes agree well for the same methods, as they should. 2) the eigenvalue by the fine–mesh diffusion calculation is ~ 6% lower than the corresponding

transport result from TWODANT. 3). Diffusion theory underestimates the power density by ~ 8% near the control rod. The differences between discrete ordinates and diffusion theory results were much less without the control rod. This example demonstrates the importance of accounting for transport effects in reactor problems.

RECENT DEVELOPMENTS

The discrete ordinates method for neutral particle transport was recently extended[7] to solve coupled photon–electron transport problems with appropriately defined cross sections to model the forward–peaked electron scattering and the continuous slowing down process. This method offers the adjoint capability and typically reduces the computing time by factors of 10 to 30 over the Monte Carlo method for the same accuracy.

Improved spatial difference schemes, collectively known as the nodal methods, have recently been developed.[16] Nodal methods augment the finite difference equations with auxiliary relations derived by preserving the spatial moments, and provide more accurate solution than the conventional finite difference methods. In a model well–logging configuration the nodal S_N method needed less than a tenth of the CPU time of the linear diamond scheme with both methods yielding a 2% accuracy in detector response.[6] In a three–dimensional concrete building shielding problem the nodal method[17] reduced the maximum error in the leakage by nearly 10–fold over the weighted difference scheme. Several hours of Cray CPU time were saved in both problems to attain the same accuracy.

Other improvements to the discrete ordinates method are incorporation of spatial finite element methods[18], extension of nodal methods to curved geometries[19,20] and time–dependent transport problems[21], and development of alternative acceleration schemes[22] applicable to higher–order spatial differencing schemes.

The major disadvantage of discrete ordinates method is the occurrence of the ray effect[23] in two and three dimensions. This arises from the discrete representation of the angular variable and can result in spurious oscillations in the flux. The ray effect is severe

in problems with strongly absorbing media or isolated sources. The procedures[23–25] to mitigate this are not fully satisfactory for they are either inadequate or too expensive. Recently, methods have been devised[26,27] to treat the angular variable by an approach similar to the multigroup approximation. These provided average particle–directions based on the flux and have been shown to reduce the ray effect.

The discrete ordinates method offers attractive features for vector and parallel processing. The spatial–mesh sweep can be vectorized[14] and parallel iterations strategies have been developed[28] with significant reduction in the CPU time.

CONCLUSIONS

The discrete ordinates method is a powerful technique to solve the Boltzmann transport equation. However, the user must be cognizant of certain limitations to apply the method effectively. It has been employed in a wide range of radiation transport problems with considerable success. Further applications are being explored by many researchers. Improvements in the associated numerical schemes have enhanced the capabilities of discrete ordinates methods to make them competitive with Monte Carlo methods for three–dimensional problems.

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Figure Captions

Figure 1. Eigenvalues and Power Profiles of the BWR Rod Bundle Problem with Cruciform Control Rod (pointwise flux convergence criterion = $2\text{x}10^{-5}$).

Multiplication Factor

	TWODANT	DORT
S2	0.645399	
S4	0.676582	0.675448 (DD/DSA)
S8	0.675446	0.675423 (WD/DSA)
S12	0.675303	
S16	0.675238	
Diffusion	0.633724	

						0.604 0.556
					1.143 1.079	0.858 0.800
				1.671 1.623	1.473 1.417	0.960 0.908
			2.108 2.082	1.865 1.833	0.658 0.660	1.213 1.166
		2.530 2.551	2.278 2.282	2.105 2.086	1.925 1.895	1.452 1.411
	3.199 3.279	2.811 2.869	0.961 0.999	2.377 2.388	2.308 2.292	1.823 1.794
S16 →	3.486	3.653	3.278	2.970	2.826	2.764	2.071
Diffusion →	3.598	3.763	3.356	3.028	2.851	2.768	2.052