6.1 The S_n Angular Discretization

So far we have covered in depth numerical methods for solving the diffusion equation. We will now begin the study of numerical methods for the solution of the transport equation. The first method we study is the discrete ordinates method, usually abbreviated as the $S_n$method. This approach solves the transport equation for the angular flux along particular directions and uses a quadrature rule to estimate integrals.

To present the $S_n$method we begin with the multigroup transport equation for a particular direction $\hat{\Omega}_n$:

where we have written the angular flux along direction $\hat{\Omega}_n$ as

$$\psi_{gn}(\mathbf{x}, t) = \psi_g(\mathbf{x}, \hat{\Omega}_n, t). \tag{6.2}$$

Also note that we have truncated the scattering order at level L.

To relate moments to angular fluxes along discrete directions we use a quadrature rule. A quadrature rule is a formula for estimating an integral by using the value of the integrand at discrete points (called ordinates) multiplied by a weight. In particular we estimate the moments in Eq. (6.1) as

$$\phi_{glm}(\mathbf{x}, t) = \int_{4\pi} d\hat{\Omega}\, Y_{lm}(\hat{\Omega})\psi_g(\mathbf{x}, \hat{\Omega}_n, t) \approx \sum_{n=1}^{N_{\text{angles}}} w_n Y_{lm}(\hat{\Omega}_n)\psi_{gn}(\mathbf{x}, t). \tag{6.3}$$

There are many different quadrature rules, or sets $\{w_n, \hat{\Omega}_n\}$, that one can use in the $S_n$method. For whichever quadrature rule one chooses, the values of w_n

and $\hat{\Omega}_n$ are known. Plugging in the quadrature rule into Eq. (6.1) gives

The boundary conditions for the $S_n$equations specify the angular flux along the incoming directions:

$$\psi_{gn}(\mathbf{x}, t) = f_g(\mathbf{x}, \hat{\Omega}_n, t), \qquad \text{for } \mathbf{x} \in \partial V \text{ and } \hat{n} \cdot \hat{\Omega}_n < 0, \tag{6.5}$$

where $\hat{n}$ is the outward normal to the boundary. Initial conditions specify the value of $\psi_{gn}(\mathbf{x}, 0)$.

Equation (6.4) defines a set of $G \times N$ partial differential equations. We can also specify an $S_n k$-eigenvalue problem as

with boundary conditions that specify either reflecting, albedo, or vacuum

boundary conditions. Alternatively, the α-eigenvalue problem is written as

6.2 Some example quadrature sets

In order to fully-specify the $S_n$equations we need to specify the quadrature set $\{w_n, \hat{\Omega}_n\}$. The quadrature directions are written as the vector

which has the property

The quadrature set also has restrictions on the ordinates. One condition we would like the set to have is that if (η_n, ξ_n, μ_n) is in the quadrature set then all eight ordinate sets $(\pm\eta_n, \pm\xi_n, \pm\mu_n)$ with the same weight on each should be included to make the set symmetric and to enable reflecting boundary conditions. This condition on the symmetry of the quadrature also implies that

We also want the weights to be normalized so that the sum of the weights should add up to 4π:

It is possible to have quadrature sets that do not have weights that add up to 4π. If this is the case we can scale the weights by a constant to make them add up to 4π. Finally, we need to have a quadrature set be able to integrate $\hat{\Omega} \otimes \hat{\Omega}$ exactly so that

Other than those conditions, we have a large amount of freedom to choose the quadrature weights and ordinates. A common approach is the level symmetric quadrature set that ensures that the points at which we evaluate μ, η, and ξ are the same (these are referred to as level symmetric quadrature sets). This leads to the condition that

$$\mu_i^2 = \mu_1^2 + \frac{2(i-1)(1-3\mu_1^2)}{N-2}, \qquad i = 1, 2, \ldots, \frac{N}{2}, \tag{6.8}$$

where N is the number of levels for μ. Note that once μ_1 is selected the other quadrature points are then defined.

Even with this constraint there is additional freedom in the quadrature set. We use this freedom to enforce the condition that any even power of a direction cosine is integrated exactly. This leads to the quadrature sets given in Table 6.1.

Another important quadrature set is called a product quadrature set. This set is motivated by the fact that integration over the unit sphere can be written as

$$\int_{4\pi} d\hat{\Omega} = \int_{-1}^{1} d\mu \int_{0}^{2\pi} d\varphi = 2 \int_{-1}^{1} d\mu \int_{-1}^{1} \frac{dy}{\sqrt{1-y^2}}, \tag{6.9}$$

where we have made the substitution $y = \cos\varphi$.

Now the integral over μ can be handled using Gauss-Legendre quadrature. The Gauss-Legendre quadrature set is a set of points and weights, $\{w_n, \mu_n\}$, that exactly integrate polynomials of degree $2N_L - 1$ over the range $\mu \in [-1, 1]$ where N_L is the number of points in the quadrature set (this means that it will exactly integrate a constant, linear, or quadratic function of μ as long as $N_L > 2$). Gauss-Legendre quadrature also is symmetric about 0 so that if μ_n

Table 6.1: The values of a level symmetric quadrature set in the first quadrant. Note $\xi_n = \sqrt{1-\mu_n^2-\eta_n^2}$.

		μ_n	η_n	w_n
S_2	1	$1/\sqrt{3}$	$1/\sqrt{3}$	1.0
S_4	1	0.350021	μ_3	1/3
	2	μ_1	μ_1	w_1
	3	0.868890	μ_1	w_1
S_6	1	0.266636	μ_6	0.176126
	2	μ_1	μ_4	0.157207
	3	μ_1	μ_1	w_1
	4	0.681508	μ_4	w_2
	5	μ_4	μ_1	w_2
	6	0.926181	μ_1	w_1
S_8	1	0.218218	μ_{10}	0.1209877
	2	μ_1	μ_8	0.0907407
	3	μ_1	μ_5	w_2
	4	μ_1	μ_1	w_1
	5	$1/\sqrt{3}$	μ_8	w_8
	6	μ_5	μ_5	0.0925927
	7	μ_5	μ_1	w_2
	8	0.786796	μ_5	w_2
	9	μ_8	μ_1	w_2
	10	0.951190	μ_1	w_1

Table 6.2: Points and weights for several orders of Gauss-Legendre Quadrature. Note only the positive μ ordinates are given because the sets are symmetric about 0.

N_L	μ_n	w_n
2	0.577350269	1
4	0.339981044	0.652145
	0.861136312	0.347855
6	0.661209386	0.360761573
	0.238619186	0.467913935
	0.932469514	0.171324492
8	0.183434642	0.362683783
	0.52553241	0.313706646
	0.796666477	0.222381034
	0.960289856	0.101228536

is in the quadrature set then $-\mu_n$ is also in the set. Some Gauss-Legendre quadrature sets are given in Table 6.2. It is common to only use even-order quadrature sets because odd order sets have $\mu = 0$ in them which presents problems in slab geometry.

The integral over y in Eq. (6.9) is treated using ChebyshevGauss quadrature. This quadrature method can exactly integrate polynomials of degree $2N_C - 1$ multiplied by $(1-y)^{-1/2}$ over the range $y \in [-1, 1]$., where N_C is the number of quadrature points. The points and weights for ChebyshevGauss quadrature are given by

$$y_n = \cos\left(\frac{2n-1}{2N_C}\pi\right), \qquad w_n = \frac{\pi}{N_C}. \tag{6.10}$$

Given that $y = \cos\varphi$, the quadrature azimuthal angles are

$$\varphi_n = \frac{2n-1}{2N_C}\pi. \tag{6.11}$$

A product quadrature then combines all the permutations of the Gauss-Legendre and Chebyshev-Gauss quadratures of the same order. The weights are the product of the weights from Gauss-Legendre and the weights from Chebyshev-Gauss. The product quadratures for orders up to 8 are given in Table 6.3.

6.2.1 Simplifications in 2-D and Slab Geometry

Many problems in nuclear reactor analysis solve the transport equation in two dimensions. In these problems there is symmetry in the solution in the z direction so we can ignore the four octants with $\mu < 0$ in our quadrature set. Our

Table 6.3: Product quadrature sets for the first octant of several orders. The number of points in each octant is $N^2/4$ for a total number of points $2N^2$.

N	n	μ_n	η_n	ξ_n	w_n
2	1	0.577350269	0.577350269	0.577350269	1.570796327
4	1	0.339981044	0.868846143	0.359887856	0.512193485
	2	0.861136312	0.194546356	0.469676451	0.273204678
	3	μ_1	η_2	ξ_2	w_1
	4	μ_2	η_1	ξ_1	w_2
6	1	0.661209386	0.900878523	0.241389673	0.188894318
	2	0.238619186	0.624922615	0.624922615	0.244999163
	3	0.932469514	0.254992316	0.951644281	0.089705294
	4	μ_1	η_2	ξ_2	w_1
	5	μ_2	η_3	ξ_3	w_2
	6	μ_3	η_1	ξ_1	w_3
	6	μ_1	η_3	ξ_3	w_1
	8	μ_2	η_1	ξ_1	w_2
	9	μ_3	η_2	ξ_3	w_3
8	1	0.183434642	0.914005834	0.181807064	0.142425589
	2	0.52553241	0.789496987	0.527525021	0.123192312
	3	0.796666477	0.541658661	0.810649474	0.087328828
	4	0.960289856	0.194088182	0.975747181	0.039752353
	5	μ_1	η_2	ξ_2	w_1
	6	μ_2	η_3	ξ_3	w_2
	7	μ_3	η_4	ξ_4	w_3
	8	μ_4	η_1	ξ_1	w_4
	9	μ_1	η_3	ξ_3	w_1
	10	μ_2	η_4	ξ_4	w_2
	11	μ_3	η_1	ξ_1	w_3
	12	μ_4	η_2	ξ_2	w_4
	13	μ_1	η_4	ξ_4	w_1
	14	μ_2	η_1	ξ_1	w_2
	15	μ_3	η_2	ξ_2	w_3
	16	μ_4	η_3	ξ_3	w_4

discrete ordinates equations are then

In 1-D slab geometry the problem changes significantly in terms of what the quadrature sets need to be. We can think of the angular flux as being azimuthally symmetric so that we can integrate over the azimuthal direction to get the slab geometry discrete ordinates equations:

For 1-D slab geometry one typically uses Gauss-Legendre quadrature to define the μ_n and w_n.

6.3 Solving Multigroup Discrete Ordinates Problems

As we saw in multigroup diffusion, all discrete ordinates problems require the solution of single-group discrete ordinates problems of the form:

We can see that steady-state, multigroup, fixed source discrete ordinates calculations can be solved using a series of steady-state, single-group, fixed source calculations by defining an iteration index ℓ and performing the Gauss-Seidel style iteration for the scattering source we discussed for diffusion:

We can cast this in the form of Eq. (6.14) by defining

$$q(\mathbf{x},\hat{\Omega}_n) = \sum_{l=0}^{L}\sum_{m=-l}^{l} Y_{lm}(\hat{\Omega}_n)\left[\sum_{g'<g}^{G}\Sigma_{slg'\rightarrow g}(\mathbf{x})\phi_{lm}^{\ell+1}(\mathbf{x}) + \sum_{g'>g}^{G}\Sigma_{slg'\rightarrow g}(\mathbf{x})\phi_{lm}^{\ell}(\mathbf{x})\right] + \frac{\chi_g(\mathbf{x})}{4\pi}\sum_{g'=1}^{G}\bar{\nu}\Sigma_{fg'}(\mathbf{x})\phi_{g'}^{\ell}(\mathbf{x},t) + q_g(\mathbf{x},\hat{\Omega}_n). \quad (6.16)$$

We can generalize this to time-dependent problems by interpreting the solution to Eq. (6.14) as the value of the angular flux at time level $m+1$ and making the change

and

$$q(\mathbf{x},\hat{\Omega}_n) = \sum_{l=0}^{L}\sum_{m=-l}^{l} Y_{lm}(\hat{\Omega}_n)\left[\sum_{g'<g}^{G}\Sigma_{\mathrm{s}lg'\to g}(\mathbf{x})\phi_{lm}^{\ell+1,m+1}(\mathbf{x}) + \sum_{g'>g}^{G}\Sigma_{\mathrm{s}lg'\to g}(\mathbf{x})\phi_{lm}^{\ell,m+1}(\mathbf{x})\right] + \frac{\chi_g(\mathbf{x})}{4\pi}\sum_{g'=1}^{G}\bar{\nu}\Sigma_{\mathrm{f}g'}(\mathbf{x})\phi_{g'}^{\ell,m+1}(\mathbf{x}) + \qquad . \quad (6.17)$$

Finally, for k-eigenvalue problems we set up each power iteration as the solution to the multigroup problem

where q_g^ℓ is the fission source

$$q_g^\ell = \frac{\chi_g(\mathbf{x})}{4\pi k_{\mathrm{eff}}}\sum_{g'=1}^{G}\bar{\nu}\Sigma_{\mathrm{f}g'}(\mathbf{x})\phi_{g'}^{\ell}(\mathbf{x}). \quad (6.19)$$

6.4 The Diamond Difference Spatial Discretization

Beginning with the slab-geometry discrete-ordinates transport equation for a single group,

(6.20)

where the moments are quadrature sums

$$\phi_l(z) = \sum_{n'=1}^{N} w'_n P_l(\mu'_n) \frac{2l+1}{2} \Sigma_{sl}(z) \psi_{n'}(z). \tag{6.21}$$

We integrate this equation over a generic zone ranging from $z_{i-1/2}$ to $z_{i+1/2}$ and divide by h_z to get for $i = 1, \ldots, I$

(6.22)

where the average over a zone is

$$(\cdot)_i = \frac{1}{h_z} \int_{z_{i-1/2}}^{z_{i+1/2}} dz \; (\cdot), \tag{6.23}$$

and the values on the edge of the zone are written as $\psi_{n,i\pm1/2}$. To relate the cell-averages to the edge values we use a simple average:

$$\psi_{ni} = \frac{1}{2}\left(\psi_{n,i+1/2} + \psi_{n,i-1/2}\right), \qquad \phi_{li} = \frac{1}{2}\left(\phi_{l,i+1/2} + \phi_{l,i-1/2}\right). \tag{6.24}$$

Equations (6.27) and (6.24) give a closed system of equations to find the cell-edge angular fluxes for the problem. Including the boundary conditions is straightforward: on the boundary for the incoming directions one uses the specified boundary condition as

$$\psi_{n,1/2} = \begin{cases} f(\mu_n) & \mu_n > 0 \\ \psi_{n,1/2} & \mu_n < 0, \end{cases} \tag{6.25}$$

$$\psi_{n,I+1/2} = \begin{cases} f(\mu_n) & \mu_n < 0 \\ \psi_{n,1/2} & \mu_n > 0. \end{cases} \tag{6.26}$$

We can generalize the diamond difference equations to 3-D as

$$\eta_n \frac{\psi_{n,i+1/2,jk} - \psi_{n,i-1/2,jk}}{h_x} + \xi_n \frac{\psi_{n,i,j+1/2,k} - \psi_{n,i,j-1/2,k}}{h_y} +$$
$$mu_n \frac{\psi_{n,ijk+1/2} - \psi_{n,ijk-1/2}}{h_z} + \Sigma_{ti} \psi_{nijk} = \sum_{l=0}^{L} \sum_{m=-l}^{l} \frac{2l+1}{2} Y_{lm}(\hat{\Omega}_n) \Sigma_{slijk} \phi_{lmijk} + q_{nijk}, \tag{6.27}$$

with

$$\psi_{nijk} = \frac{1}{6}\left(\psi_{n,i+1/2,jk} + \psi_{n,i-1/2,jk} + \psi_{n,i,j+1/2,k} + \psi_{n,i,j-1/2,k} + \psi_{n,ijk+1/2} + \psi_{n,ijk-1/2}\right). \tag{6.28}$$