Lecture 17

Equivalence of the S_N and P_{N-1} Methods

The purpose of this lecture is to demonstrate that the 1-D slab-geometry S_N equations with Gauss quadrature and a Legendre cross section expansion of degree $N-1$ are equivalent to the P_{N-1} equations. We begin with the S_N equations:

$$\mu_m \frac{\partial \psi_m}{\partial x} + \sigma_t \psi_m = \sum_{k=0}^{N-1} \frac{2k+1}{4\pi} \left(\sigma_k \phi_k + q_k\right) P_k(\mu_m)\,, \quad m = 1, N. \tag{1}$$

Multiplying Eq. (1) by $P_n(\mu_m)$ and using the following recursion relationship,

$$\mu P_n(\mu) = \frac{n+1}{2n+1} P_{n+1}(\mu) + \frac{n}{2n+1} P_{n-1}(\mu)\,, \tag{2}$$

we obtain

$$\begin{aligned} &\frac{\partial \psi_m}{\partial x} \left[\frac{n+1}{2n+1} P_{n+1}(\mu_m) + \frac{n}{2n+1} P_{n-1}(\mu_m) \right] + \sigma_t \psi_m P_n(\mu_m) = \\ &\qquad \sum_{k=0}^{N-1} \frac{2k+1}{4\pi} \left(\sigma_k \phi_k + q_k\right) P_k(\mu_m) P_n(\mu_m)\,, \quad m = 1, N. \end{aligned} \tag{3}$$

Using the Gauss quadrature to integrate Eq. (3) over all directions, we get

$$\begin{aligned} &\frac{n+1}{2n+1} \frac{\partial}{\partial x} \langle \psi P_{n+1} \rangle + \frac{n}{2n+1} \frac{\partial}{\partial x} \langle \psi P_{n-1} \rangle + \sigma_t \langle \psi P_n \rangle = \\ &\qquad \sum_{k=0}^{N-1} \frac{2k+1}{4\pi} \left(\sigma_k \phi_k + q_k\right) \langle P_k P_n \rangle\,, \quad m = 1, N, \end{aligned} \tag{4}$$

where $\langle\cdot\rangle$ denotes quadrature integration over angle. Remembering that a Gauss S_N set exactly integrates all polynomials through degree $2N-1$, and that

$$2\pi \int_{-1}^{+1} P_n(\mu) P_k(\mu)\, d\mu = \frac{4\pi}{2k+1}\delta_{n,k}\,, \tag{5}$$

Eq. (4) reduces to the following two equations:

$$\frac{n+1}{2n+1}\frac{\partial \phi_{n+1}}{\partial x} + \frac{n}{2n+1}\frac{\partial \phi_{n-1}}{\partial x} + (\sigma_t - \sigma_n)\,\phi_n = q_n\,, \quad n = 0, N-2, \tag{6a}$$

$$\frac{N}{2N-1}\frac{\partial \phi_N}{\partial x} + \frac{N-1}{2N-1}\frac{\partial \phi_{N-2}}{\partial x} + (\sigma_t - \sigma_{N-1})\,\phi_{N-1} = q_{N-1}\,. \tag{6b}$$

Equations (6a) and (6b) are the P_{N-1} equations provided that $\phi_N = 0$ To demonstrate that this is in fact the case, we note that the Gauss points for an N-point quadrature are the roots of $P_N(\mu)$. Thus,

$$P_N(\mu_m) = 0\,, \quad m = 1, M, \tag{7}$$

and

$$\phi_N = \sum_{m=1}^{N} \psi_m P_N(\mu_m) w_m = 0\,, \tag{8}$$

so Eq. (6b) is actually the correct equation for ϕ_{N-1}:

$$\frac{N-1}{2N-1}\frac{\partial \phi_{N-2}}{\partial x} + (\sigma_t - \sigma_{N-1})\,\phi_{N-1} = q_{N-1}\,. \tag{9}$$

This completes the demonstration that the 1-D slab-geometry S_N equations with Gauss quadrature and a Legendre cross-section expansion of degree $N-1$ are equivalent to the

P_{N-1} equations. However, this does not necessarily imply that the S_N and P_{N-1} equations give the same solutions. This will only be the case if the boundary conditions are equivalent. We have previously discussed only Marshak conditions for the P_n equations. The S_N boundary conditions are equivalent to Mark boundary conditions for the P_{N-1} equations. These conditions are defined for the P_{N-1} equations in terms of the Gauss S_N quadrature points and they require that the exact boundary conditions be approximately met via collocation at the quadrature points. For instance let $\tilde{\psi}$ denote the Legendre expansion for the angular flux associated with the P_{N-1} approximation:

$$\tilde{\psi} = \sum_{n=0}^{N-1} \frac{2n+1}{4\pi} \phi_n P_n(\mu)\,, \tag{10}$$

and let $f(\mu)$ denote the incident flux at a boundary. The Mark reflective condition requires that $\tilde{\psi}(\mu) = \tilde{\psi}(-\mu)$ at the Gauss quadrature points. The Mark and Marshak reflective conditions are equivalent. The Mark source condition formally requires that $\tilde{\psi}(\mu) = f(\mu)$ at the incoming Gauss quadrature points. However, if this is done, the solution will not be conservative. To ensure conservation, two modifications are required. The first is to renormalize the point values of f to ensure the correct incoming current using Gauss quadrature. For instance, at the left boundary, one defines the Mark boundary condition as follows:

$$\tilde{\psi}(\mu_m) = \sum_{n=0}^{N-1} \frac{2n+1}{4\pi} \phi_n P_n(\mu_m) = f^*(\mu_m), \quad \mu_m > 0, \tag{11}$$

where the point values of f are renormalized to yield the exact incoming current using Gauss quadrature:

$$f^*(\mu_m) = f(\mu_m) \frac{2\pi \int_{-1}^{+1} f(\mu)\mu \, d\mu}{\sum_{\mu_k>0} f(\mu_k)\mu_k w_k} \,. \tag{12}$$

The second is to compute the outgoing current using Gauss quadrature:

$$j^- = -\sum_{\mu_m<0} \tilde{\psi}(\mu_m)\mu_m w_m \,. \tag{13}$$

As required, the Mark conditions impose $N/2$ equations at each boundary.

The Marshak and Mark source conditions are not equivalent. To give the reader some perspective in this regard, we consider the P_1 case. The Gauss S_2 quadrature points are $\mu = \pm 1/\sqrt{3}$ with each point having a weight of 2π. The Mark source condition at the left boundary is given by

$$\left[\frac{\phi}{4\pi} + \frac{3}{4\pi} J \frac{1}{\sqrt{3}}\right] \frac{1}{\sqrt{3}} 2\pi = 2\pi \int_{-1}^{+1} f(\mu)\mu \, d\mu \equiv j^+ \,. \tag{14}$$

If we put Eq. (4) in the form of an extrapolated boundary condition, we get

$$\phi - \sqrt{3} D \frac{\partial \phi}{\partial x} = 2\sqrt{3} j^+ \,. \tag{15}$$

The above expression is to be contrasted with that corresponding to the Marshak condition:

$$\phi - 2D \frac{\partial \phi}{\partial x} = 4 j^+ \,. \tag{16}$$

Comparing Eqs. (15) and (16), we find that the extrapolation distance is $\sqrt{3}D$ for the Mark condition but $2D$ for the Marshak condition, and the extrapolated flux value is

$2\sqrt{3}j^+$ for the Mark condition but $4j^+$ for the Marshak condition. It can be shown that for the half-space problem with an incident half-range current of j^+ and $\sigma_t = \sigma_s$, the Marshak condition yields the exact solution of $\phi = 4j^+$, whereas the Mark condition yields a solution of $2\sqrt{3}j^+$ with an error of roughly 15 percent. On the other hand, it can be shown that for the half-space problem with an incident half-range current of j^+ and $\sigma_t = \sigma_a$, the Marshak condition yields the erroneous and non-physically negative reflected fraction of $j^-/j^+ = (1-2/\sqrt{3})/(1+2/\sqrt{3})$, whereas the Mark condition yields the exact value of zero. The difference between P_n solutions obtained with Marshak conditions and those obtained with Mark conditions rapidly decreases with increasing n.