Lecture 14

The P_n or Spherical–Harmonics Approximation

1 Derivation of the Equations

We previously derived the diffusion equation by applying a Galerkin approximation based on a linear angular trial space and weighting space. The P_n approximation represents a generalization of this concept based on higher–order polynomial trial spaces. We begin this discussion by considering the Legendre polynomials.

The Legendre polynomials, $\{P_n(x)\}_{n=0}^{\infty}$, are defined over the interval $[-1,+1]$ and form an orthogonal basis set for the space of polynomials on that interval. They also represent the associated Legendre functions of order zero, as discussed in Appendix C. Two of the properties of the Legendre polynomials that we will use are as follows:

$$\int_{-1}^{+1} P_n(\mu)\; P_m(\mu)\, d\mu = \frac{2}{2n+1}\; \delta_{n,m}\,, \tag{1}$$

and

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

where

$$P_0(\mu) = 1\,, \tag{3}$$

$$P_1(\mu) = \mu\,. \tag{4}$$

We begin the derivation of the P_n equations by considering the 1-D slab–geometry transport equation with anisotropic scattering and an anisotropic distributed source. We assume infinite-order Legendre expansions for both sources:

$$\mu\frac{\partial\psi}{\partial x} + \sigma_t\psi = \sum_{n=0}^{\infty}\frac{2n+1}{4\pi}\left(\sigma_n\phi_n + q_n\right)P_n(\mu)\,, \tag{5}$$

where the Legendre moments of the scattering cross-section are given by

$$\sigma_n = 2\pi\int_{-1}^{+1}\sigma_s(\mu_0)P_n(\mu_0)\,d\mu_0\,, \tag{6}$$

and the Legendre moments of the angular flux are given by

$$\phi_n = 2\pi\int_{-1}^{+1}\psi(\mu)P_n(\mu)\,d\mu\,. \tag{7}$$

Next we assume a trial space expansion of the following form:

$$\psi(x,\mu) = \sum_{n=0}^{N}\frac{2n+1}{4\pi}\phi_n(x)P_n(\mu)\,, \tag{8}$$

where N is odd. The reason for doing this is explained later. Equations for the expansion coefficients, $\{\phi_\ell\}_{\ell=0}^{N}$, can be obtained by substituting from Eq. (8) into Eq. (5), successively multiplying that equation by $P_0(\mu)$, $P_1(\mu)$, $\ldots P_N(\mu)$, and integrating over all directions. In particular, substituting from Eq. (8) into Eq. (5), we get

$$\mu\frac{\partial}{\partial x}\sum_{n=0}^{N}\frac{2n+1}{4\pi}\phi_n P_n(\mu) + \sigma_t\sum_{n=0}^{N}\frac{2n+1}{4\pi}\phi_n P_n(\mu) =$$

$$\sum_{n=0}^{N} \frac{2n+1}{4\pi} \sigma_n \phi_n P_n(\mu) + \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} q_n P_n(\mu)\,. \tag{9}$$

Note that the scattering source expansion is truncated at $n = N$ in Eq. (9) because Eq. (8) implies that

$$\phi_n = 0\,, \quad n > N. \tag{10}$$

Substituting from Eq. (2) into Eq. (9), we get

$$\frac{\partial}{\partial x} \sum_{n=0}^{N} \frac{2n+1}{4\pi} \phi_n \left(\frac{n+1}{2n+1} P_{n+1}(\mu) + \frac{n}{2n+1} P_{n-1}(\mu) \right) +$$

$$\sigma_t \sum_{n=0}^{N} \frac{2n+1}{4\pi} \phi_n P_n(\mu) = \sum_{n=0}^{N} \frac{2n+1}{4\pi} \sigma_n \phi_n P_n(\mu) + \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} q_n P_n(\mu)\,. \tag{11}$$

Multiplying Eq. (11) by $\mathrm{P}_k(\mu)$, where $0 \le k \le N$, integrating over all directions, and using the orthogonality condition given in Eq. (1), we obtain

$$\frac{k}{2k+1} \frac{\partial \phi_{k-1}}{\partial x} + \frac{k+1}{2k+1} \frac{\partial \phi_{k+1}}{\partial x} + (\sigma_t - \sigma_k)\, \phi_k = q_k \quad k = 0, N. \tag{12}$$

Evaluating Eq. (12), for $k = 0$, we get

$$\frac{\partial \phi_1}{\partial x} + (\sigma_t - \sigma_0)\, \phi_0 + q_0\,. \tag{13}$$

Taking Eqs. (3), (4), (6), and (7) into account, it follows that $\phi_0 = \phi$, $\phi_1 = J$, and $\sigma_0 = \sigma_s$. Thus Eq. (13) is seen to be the balance equation:

$$\frac{\partial J}{\partial x} + \sigma_a \phi = q_0\,. \tag{14}$$

Evaluating Eq. (12) for $k = N$ and taking Eq. (11) into account, we get

$$\frac{N}{2N+1}\frac{\partial \phi_{N-1}}{\partial x} + (\sigma_t - \sigma_N)\,\phi_N = q_N \,. \tag{15}$$

Thus for the P_n approximation of degree N, Eq. (13) represents the equation for ϕ_0, Eq. (12) represents the equation for ϕ_k, with $0 < k < N$, and Eq. (15) represents the equation for ϕ_N. Each of these equations is exact except for Eq. (15). The exact equation for ϕ_N follows from Eq. (12):

$$\frac{N}{2N+1}\frac{\partial \phi_{N-1}}{\partial x} + \frac{N+1}{2k+1}\frac{\partial \phi_{N+1}}{\partial x} + (\sigma_t - \sigma_N)\,\phi_N = q_N \,, \tag{16}$$

which contains ϕ_{N+1}. The system of exact moment equations through degree N is not closed because there are $N+2$ unknowns and only $N+1$ equations. The closure, $\phi_{N+1} = 0$, follows from Eq. (8). There are other possible closures leading to generalized P_n methods, but we will not discuss them here.

2 Boundary Conditions

In general, the boundary conditions for the angular flux cannot be met exactly with a global polynomial trial space. Thus the boundary conditions must be met approximately. This is analogous to the case of diffusion theory. It follows from Eqs. (3), (4), and (8), that the P_1 approximation is identical to the diffusion approximation for the steady-state case. Thus

Marshak conditions can be used for the P_1 equations (this is so for the time-dependent case as well.) The central theme of the Marshak condition for diffusion theory is to preserve the incoming current. This theme is generalized for the P_N case to preservation of the even Legendre moments of the incoming current. For instance, assuming an incident flux on the left boundary denoted by $f_L(\mu)$, the Marshak condition requires that

$$2\pi \int_0^{+1} \left[\sum_{n=0}^{N} \frac{2n+1}{4\pi} \phi_n(x_L) P_n(\mu) \right] \mu P_k(\mu)\, d\mu =$$
$$2\pi \int_0^{+1} f_L(\mu) \mu P_k(\mu)\, d\mu\,, \quad k = 0, 2, \ldots, N-1. \tag{17}$$

Marshak vacuum conditions are obtained simply by setting the incident flux to zero in Eq. (17). For the case of a reflective condition, one simply sets the odd Legendre moments to zero. For instance, for a reflective condition at the left boundary, one requires that

$$\phi_k(x_L) = 0\,, \quad k = 1, 3, \ldots, N. \tag{18}$$

As in the case of the diffusion approximation, these are the only reflective conditions that are physically acceptable. At a material interface, each Legendre flux moment must be continuous across the interface. As in the case of reflection, these are the only interface conditions that are physically acceptable.

The Marshak source and vacuum conditions, and the reflective conditions each provide $(N+1)/2$ equations at a boundary. The total number of boundary equations is thus $N+1$. This closes the system of equations since there are $N+1$ first–order equations. We do not consider the P_N approximation with N an even number because this forces an unnatural asymmetry in the boundary conditions, i.e., one boundary must have one more condition than the other.

Equation (17) clearly represents a straight-forward generalization of the Marshak condition for the diffusion equation, and Eq. (18) similarly represents a straight-forward generalization of the reflective condition for the diffusion equation. However, in the higher-order case ($N > 1$), the Marshak condition cannot be interpreted in terms of a boundary extrapolation.

There are many types of source boundary conditions other than the Marshak conditions that can be used with the P_n equations. However, we will not discuss them here since those significantly more accurate than the Marshak conditions require knowledge of the transport solution. Furthermore, the P_n solution converges to the transport solution as n is increased with any valid boundary conditions. Thus the sensitivity of the solution to the type of boundary conditions used is much less important for a high-order solution than for a low-order solution.