**NE 155/255, Fall 2019**
**Discrete Ordinates**
**October 02, 2019**

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# Angular Discretization, Continued

Recall this substitution in order to satisfy the orthogonality requirement:

$$\hat{Y}^e_{lm} = \frac{1}{\sqrt{2-\delta_{m0}}} Y^e_{lm}\,, \quad \hat{Y}^o_{lm} = \frac{1}{\sqrt{2-\delta_{m0}}} Y^o_{lm}\,. \tag{1}$$

Because $\hat{Y}^o_{\ell 0} = 0$ based on the inclusion of $\sin(m\varphi)$ in its definition, the above sometimes neglects the $\delta_{m0}$ term in the odd function since it is implied that $m = 0$ leads to an identically zero function anyways.

Next, we expand the Spherical Harmonics into real and imaginary components. The sum over $m > 0$ then becomes

$$\sum_{m=1}^{l} \Big( \hat{Y}^e_{\ell m}(\hat{\Omega})\hat{Y}^e_{\ell m}(\hat{\Omega}') + \hat{Y}^o_{\ell m}(\hat{\Omega})\hat{Y}^o_{\ell m}(\hat{\Omega}') + \hat{Y}^e_{\ell -m}(\hat{\Omega})\hat{Y}^e_{\ell -m}(\hat{\Omega}') + \hat{Y}^o_{\ell -m}(\hat{\Omega})\hat{Y}^o_{\ell -m}(\hat{\Omega}') \Big)\,, \tag{2}$$

where the imaginary terms have been set to zero because our values must be real.

Next, we use these relationships to get rid of the $-m$ terms:

$$\hat{Y}^e_{\ell -m} = (-1)^{-m}\hat{Y}^e_{\ell m} \equiv (-1)^m \hat{Y}^e_{\ell m} \text{ and} \tag{3}$$

$$\hat{Y}^o_{\ell -m} = -(-1)^m \hat{Y}^o_{\ell m}\,, \tag{4}$$

and then the summation becomes

$$\sum_{m=1}^{l} \Big( 2\hat{Y}^e_{\ell m}(\hat{\Omega})\hat{Y}^e_{\ell m}(\hat{\Omega}') + 2\hat{Y}^o_{\ell m}(\hat{\Omega})\hat{Y}^o_{\ell m}(\hat{\Omega}') \Big). \tag{5}$$

After applying these equations in the $m > 0$ terms and combining with the $m = 0$ term described above, the expression for $P_\ell(\hat{\Omega} \cdot \hat{\Omega}')$ is

$$P_\ell(\hat{\Omega}' \cdot \hat{\Omega}) = \frac{4\pi}{2\ell+1}\Big[Y^e_{\ell 0}(\hat{\Omega})Y^e_{\ell 0}(\hat{\Omega}') + \sum_{m=1}^{\ell}\big(Y^e_{\ell m}(\hat{\Omega})Y^e_{\ell m}(\hat{\Omega}') + Y^o_{\ell m}(\hat{\Omega})Y^o_{\ell m}(\hat{\Omega}')\big)\Big]\,. \tag{6}$$

Here we have replaced the $\hat{Y}$ terms with their respective definitions so that we are once again working in terms of regular spherical harmonics.

**Representing Sources with Spherical Harmonics**

We can use these terms to expand our scattering and external sources (adding energy indexing back in) for multi-D and any degree of anisotropy. We define the **scattering source** as:

$$Q^g_s(\vec{r},\hat{\Omega}) = \sum_{g'=0}^{G-1}\sum_{\ell=0}^{N}\frac{2\ell+1}{4\pi}\Sigma^{g'\to g}_{s,\ell}(\vec{r})\int_{4\pi} d\hat{\Omega}'\, P_\ell(\hat{\Omega}\cdot\hat{\Omega}')\psi^{g'}(\vec{r},\hat{\Omega}') \tag{7}$$

$$Q^g_s(\vec{r},\hat{\Omega}) = \sum_{g'=0}^{G-1}\sum_{\ell=0}^{N}\Sigma^{g'\to g}_{s,\ell}(\vec{r})\Big[Y^e_{\ell 0}(\hat{\Omega})\phi^{g'}_{\ell 0}(\vec{r}) + \sum_{m=1}^{\ell}\big(Y^e_{\ell m}(\hat{\Omega})\phi^{g'}_{\ell m}(\vec{r}) + Y^o_{\ell m}(\hat{\Omega})\vartheta^{g'}_{\ell m}(\vec{r})\big)\Big]\,, \tag{8}$$

where

$$\phi^g_{\ell m} = \int_{4\pi} Y^e_{\ell m}(\hat{\Omega})\psi^g(\hat{\Omega})\,d\hat{\Omega}\,, \quad m \geq 0\,, \tag{9}$$

$$\vartheta^g_{\ell m} = \int_{4\pi} Y^o_{\ell m}(\hat{\Omega})\psi^g(\hat{\Omega})\,d\hat{\Omega}\,, \quad m > 0\,. \tag{10}$$

Equation (8) is the multigroup anisotropic scattering source that is defined by the order of the Legendre expansion, $P_N$, of the scattering. For a given $P_N$ order, $(N+1)^2$ moments are required to integrate the scattering operator. The moments in Eqs. (9) and (10) are the *angular flux moments* or, simply, flux moments.

Applying the same methodology gives the expansion of the **external source**:

$$Q^g_e(\vec{r},\hat{\Omega}) = \sum_{\ell=0}^{N}\Big[Y^e_{\ell 0}(\hat{\Omega})q^g_{\ell 0}(\vec{r}) + \sum_{m=1}^{\ell}\big(Y^e_{\ell m}(\hat{\Omega})q^g_{\ell m}(\vec{r}) + Y^o_{\ell m}(\hat{\Omega})s^g_{\ell m}(\vec{r})\big)\Big]\,, \tag{11}$$

where the spatial dependence has been suppressed. The even and odd source moments are defined as

$$q^g_{\ell m} = \int_{4\pi} Y^e_{\ell m}(\hat{\Omega}) q^g_e(\hat{\Omega})\, d\hat{\Omega}\,, \quad m \geq 0\,, \tag{12}$$

$$s^g_{\ell m} = \int_{4\pi} Y^o_{\ell m}(\hat{\Omega}) q^g_o(\hat{\Omega})\, d\hat{\Omega}\,, \quad m > 0\,. \tag{13}$$

**Discrete Ordinates Equations**

We put all of that together to get

$$\begin{aligned}
&\hat{\Omega}_a \cdot \nabla \psi^g_a(\vec{r}) + \Sigma^g_t(\vec{r})\psi^g_a(\vec{r}) = \\
&\qquad \sum_{g'=0}^{G-1}\sum_{\ell=0}^{N} \Sigma^{g'\to g}_{s,\ell}(\vec{r}) \Big[ Y^e_{l0}(\hat{\Omega})\phi^{g'}_{\ell 0}(\vec{r}) + \sum_{m=1}^{\ell} \big( Y^e_{\ell m}(\hat{\Omega})\phi^{g'}_{\ell m}(\vec{r}) + Y^o_{\ell m}(\hat{\Omega})\vartheta^{g'}_{\ell m}(\vec{r}) \big) \Big] \\
&\qquad + \sum_{\ell=0}^{N} \Big[ Y^e_{\ell 0}(\hat{\Omega}) q^g_{\ell 0}(\vec{r}) + \sum_{m=1}^{\ell} \big( Y^e_{\ell m}(\hat{\Omega}) q^g_{\ell m}(\vec{r}) + Y^o_{\ell m}(\hat{\Omega}) s^g_{\ell m}(\vec{r}) \big) \Big]
\end{aligned}$$

The $S_N$ method will be conservative if the quadrature set effectively integrates the even and odd Spherical Harmonics.

The thing that you solve for is the flux moments, and then you reconstruct that flux at the end.

**Azimuthal Symmetry**

This all gets simpler if we have azimuthal symmetry. In that case, $m = 0$ and

$$Y_{\ell 0}(\theta, \varphi) = (-1)^0 \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-0)!}{(\ell+0)!}}\, P_{\ell 0}(\cos\theta) \mathrm{e}^{i0\varphi} = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos\theta),$$

then

$$
\begin{aligned}
&\hat{\Omega}_a \cdot \nabla \psi_a^g(\vec{r}) + \Sigma_t^g(\vec{r})\psi_a^g(\vec{r}) \\
&\qquad = \sum_{g'=0}^{G}\sum_{\ell=0}^{N} \Sigma_{s,\ell}^{g'\to g}(\vec{r})\big(Y_\ell^e(\hat{\Omega})\phi_\ell^{g'}(\vec{r})\big) + \sum_{\ell=0}^{N}\big(Y_\ell^e(\hat{\Omega})q_\ell^g(\vec{r})\big) \\
&\qquad = \sum_{g'=0}^{G}\sum_{\ell=0}^{N} \Sigma_{s,\ell}^{g'\to g}(\vec{r})\left[\sqrt{\frac{2\ell+1}{4\pi}}P_\ell(\cos\theta)\phi_\ell^{g'}(\vec{r})\right] + \sum_{l=0}^{N}\left[\sqrt{\frac{2\ell+1}{4\pi}}P_\ell(\cos\theta)q_\ell^g(\vec{r})\right]
\end{aligned}
$$

which is equivalent to what we did in the simplification class.

## Discrete Ordinates Considerations

Two main things to consider in discrete ordinates: *quadrature choice* and *ray effects*.

**Level-symmetric** quadratures use the same set of $N/2$ positive values of direction cosines with respect to each of the three axes. That is, for each level $n$ we set $\mu_a = \eta_a = \xi_a$. We describe a level $a$ as the ordinate set that has cosine $\mu_a$ with respect to the $x$-axis. Note that with this setup no axis has preferential treatment. Figure 1 shows $S_6$. We see there are $6/2 = 3$ values of each direction cosine, and each one is the same with respect to each axis. We have $N(N+2)$ quadrature points over the sphere, and that divided by 8 per octant (in this case 48 and 6, respectively).

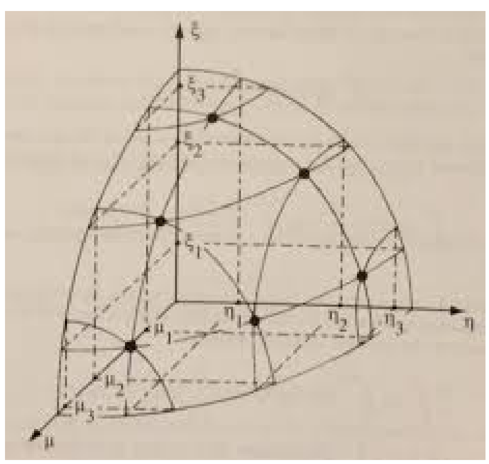


Figure 1: $S_6$ quadrature

Because of the symmetry constraints, not all of the $\mu_n$ are independent. In fact, there is only one degree of freedom because of all of the constraints. Choosing $\mu_1$ sets all of the other values as follows:

$$\mu_i^2 = \mu_1^2 + \frac{2(1 - 3\mu_1^2)}{N - 2}(i - 1) \; .$$

See 4-2 of Lewis and Miller for details. Selecting a $\mu_1$ near the poles will cause clustering at the poles, and so on.

Further, we need to select weights to perform the integration. These meet the requirement

$$\sum_{a=1}^{N(N+2)/8} w_a = 1 \; .$$

In the $S_2$ approximation, we only have one choice. For higher values we still have some choices.

A common choice is to choose weights and angles that correctly integrate as many Legendre Polynomials as possible. These are shown in in Table 4-1 in L&M and are technically called the $LQ_N$ set. There are other $S_N$ versions that have reduced symmetry or relaxation of requirements in other ways. For example, if we don't require all of the cosines to lie on the $N/2$ levels we can maintain rotational symmetry and have equal weights.