NE 155/255, Fall 2019
Discrete Ordinates, $\mathbf{P}_N$, $\mathbf{SP}_N$
October 07, 2019

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 μ_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).

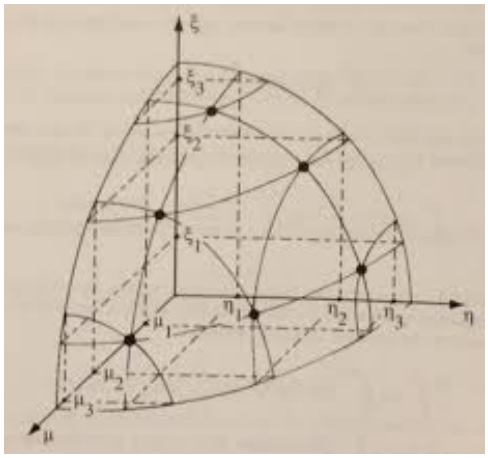


Figure 1: S_6 quadrature

Because of the symmetry constraints, not all of the μ_n are independent. In fact, there is only one degree of freedom because of all of the constraints. Choosing μ_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 μ_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.

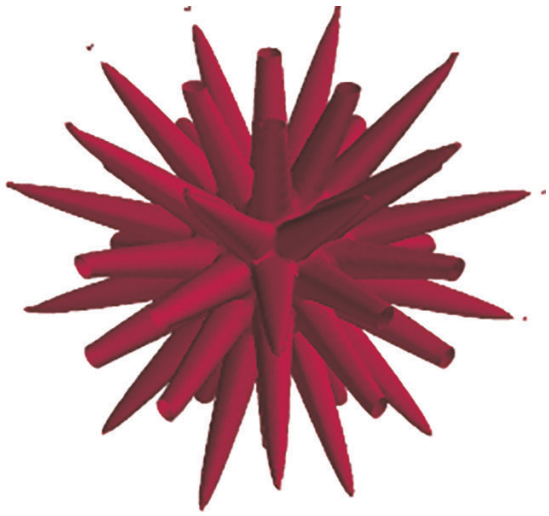
Another common quadrature is **Gauss-Legendre**. An n-point Gaussian quadrature rule is constructed to yield an exact result for polynomials of degree $2n-1$ or less by a suitable choice of the points x_i and weights w_i for $i = 1, \ldots, n$. Common weighting functions include $w(x) = 1/\sqrt{1-x^2}$ (Chebyshev-Gauss) and $w(x) = e^{-x^2}$ (Gauss-Hermite). In general, the n-th polynomial normalized to give $P_n(1) = 1$, the i-th Gauss node, x_i, is the i-th root of P_n; its weight is given by

$$w_i = \frac{2}{(1-x_i^2)\left[P_n'(x_i)\right]^2}.$$

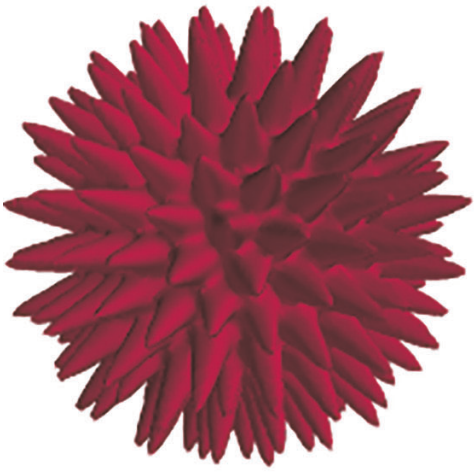
Ray Effects: ray effects come from the fact that the discrete ordinates method is exact at particular angles, but we cannot say anything about the accuracy at points off of those angles. Consider a point source in a large medium of helium gas. Consider that you've chosen S_2. What is the flux going to look like? Consider now that you've chosen S_{14}. What will the flux look like now? It is not very accurate in either case because there is nothing to scatter the neutrons from the angles in question. These are ray effects; example plots are shown on the following page.

There are "fix-up" solutions to deal with this. The best approach is probably generating a first collided flux, stopping the calculation, and starting again with the first collision source as the source. This takes the point source, smears it across the space, and allows a diffuse starting source. This functionally improves quite a bit over straight S_N in situations that have unfavorable transport characteristics.

(a)



(b)



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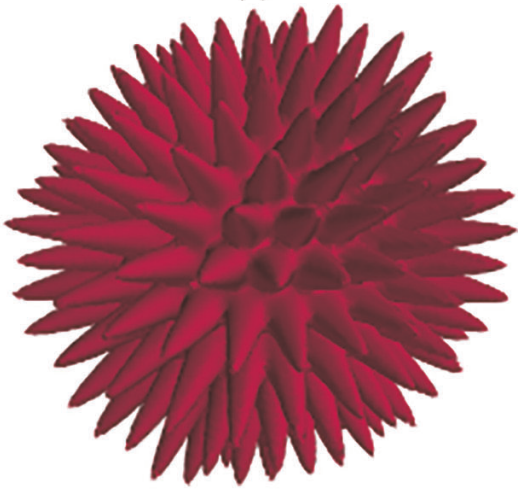

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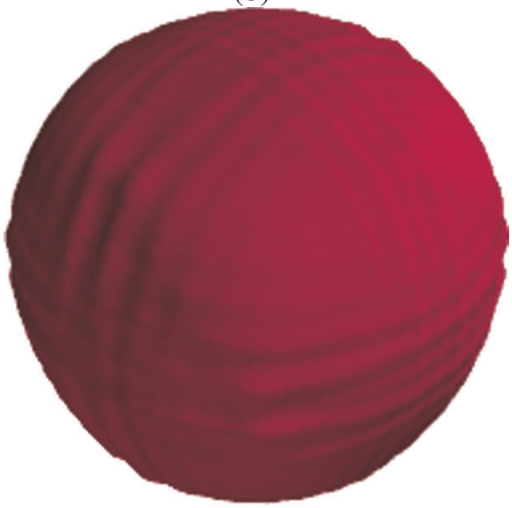

(b)

Spherical Harmonics, P_N Method

As mentioned, the other approach is using Spherical Harmonics more broadly. In this method we expand not only scattering and the sources in spherical harmonics, but the flux itself.

We use

$$\psi(x,\mu) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{4\pi} \phi_\ell(x) P_\ell(\mu)$$

for the flux solution in total in 1-D. There are some major *deficiencies* of P_N methods - e.g., we get poor representation of ψ near vacuum boundaries.

SP_N Equations (general notes)

The SP_N equations can be understood as a "super" diffusion theory. The structure of the SP_N equations is that of a coupled system of diffusion equations, and the class of problems for which the SP_N equations are accurate encompasses those for which diffusion theory is accurate.

1. In 1-D planar geometry, SP_N and P_N are identical
2. In multi-D, SP_N form a system of (N + 1) eqs; P_N form a system of $(N + 1)^2$ eqs
3. The SP_N equations have a "diffusion" (elliptic) structure; the P_N equations have a more complicated (hyperbolic) mathematical structure.
4. In principle, the 2-D or 3-D SP_N equations can be implemented in a 2-D or 3-D diffusion code without fundamentally rewriting the code. This is not the case for the P_N equations.
5. The SP_N equations contain more "transport physics" than the diffusion equations. For this reason, solutions of the SP_N equations can contain boundary layers that are not present in P_1 solutions. In order to properly resolve these boundary layers, it may be necessary to use a finer spatial grid for the SP_N equations than for the diffusion equation.
6. In the limit as $N \to \infty$, the P_N solutions converge to the transport solution.
7. In the limit as $N \to \infty$, the SP_N solutions don't generally converge to the transport solution unless the underlying problem is 1-D. Thus, high-order SP_N equations cannot be used to obtain arbitrarily accurate solutions of neutron transport problems in 2- or 3-D.

8. For 3-D problems, the system of P_N equations is much more complicated in structure and greater in number than the system of SP_N equations. Also, for problems having 1-D symmetry, the P_N and SP_N equations become identical. For these reasons, it is widely believed that the 3-D SP_N equations can be derived by discarding the proper terms (and equations) from the 3-D P_N equations. However, this has never been shown and the precise relationship between the 3-D P_N and the 3-D SP_N equations is not known.

Approximation Errors

With discrete ordinates, errors can be removed through spatial integration. The physical oscillations in the flux will balance out, and the magnitudes are pretty correct. Further, you can visually see ray effects–so you can tell that something is going on. You can increase the order, and you can see what might or might not be trustworthy.

With P_N the errors are often in magnitude rather than shape, so it is much more difficult to assess whether your solution is correct. (in complex geometries it is also sometimes hard to tell for ray effects).