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Advanced quadratures for three-dimensional discrete ordinate transport simulations: A comparative study

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A B S T R A C T

Three-dimensional radiation transport simulations play a key role in a number of problems found in nuclear science and engineering. When considering deterministic methods for solving the three-dimensional radiation transport equation, the S_n method of Carlson and Lee is one of the most commonly found techniques. The S_n method relies on a given set of "discrete ordinates" or discrete directions in which radiation streams. This set of discrete ordinates also must form a quadrature (numerical integration) so that the angular flux moments can be estimated and the scattering source calculated. In this paper we review a number of recently developed angular quadrature sets and compare their performance on a number of reactor physics problems.

1. Introduction

With the increasing availability of large computing resources, three-dimensional deterministic radiation transport simulations are becoming more commonplace, but still far from routine. One class of techniques for solving the three-dimensional radiation transport equation is based on the "angular segmentation" or S_n method of Carlson and Lee (1961). For the steady-state, monoenergetic transport problem

$$\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},\mathbf{\Omega})+\Sigma_t(\mathbf{r})\psi(\mathbf{r},\mathbf{\Omega})=\int_{\mathbb{S}^2}\Sigma_s(\mathbf{r},\mathbf{\Omega},\mathbf{\Omega}')\psi(\mathbf{r},\mathbf{\Omega}')d^2\Omega'+S(\mathbf{r},\mathbf{\Omega}) \tag{1}$$

the S_n equations read (Lewis and Miller, 1993)

$$\mathbf{\Omega}_i\cdot\nabla\psi_i(\mathbf{r})+\Sigma_t\psi_i(\mathbf{r})=\sum_{n=0}^{N}\sigma_s^n\sum_{|m|\leqslant n}\phi_n^m(\mathbf{r})Y_n^m(\mathbf{\Omega}_i)+S(\mathbf{r},\mathbf{\Omega}_i),\quad i=1,2,\ldots,M, \tag{2}$$

where the Legendre scattering moments, σ_s^n, have been truncated to degree N, ϕ_n^m are the angular flux moments, calculated by quadrature as

$$\phi_n^m(\mathbf{r})=\int_{\mathbb{S}^2}\overline{Y}_n^m(\mathbf{\Omega})\psi(\mathbf{r},\mathbf{\Omega})\approx\sum_{i=1}^{M}w_i\overline{Y}_n^m(\mathbf{\Omega}_i)\psi(\mathbf{r},\mathbf{\Omega}_i), \tag{3}$$

with Y_n^m a spherical harmonic of degree n and order m and the over bar denotes complex conjugation. The directions $\mathbf{\Omega}_i$ in Eq. (2) are from the quadrature set $\{\mathbf{\Omega}_i,w_i\}_{i=1}^M$ used in Eq. (3). Thus we see that quadratures play a central role in S_n methods. In particular, for three-dimensional S_n transport calculations, quadratures on the sphere are of particular interest.

When Carlson and Lee first developed the S_n method, they constructed the so-called level symmetric quadrature sets. These quadratures sets, a mainstay in many of today's production transport codes, were constructed using a specific prescription for the geometric placement of the nodes (directions). The associated quadrature weights were then determined by enforcing angular moment conditions and solving a linear system of equations (Carlson and Lee, 1961). Unfortunately, this construction yields negative weight quadratures when higher order quadratures are sought. Level symmetric quadratures do, however, posses cubic symmetry which is important for implementing reflective boundary conditions.

There are a number of recently developed quadratures with properties that are significantly different from the standard level-symmetric quadratures. The purpose of this paper is to report our findings from a systematic comparison, based on various reactor physics test problems, of these new quadratures.

The outline of this paper is as follows. In the first section, we outline the basic problem of constructing a quadrature on the sphere. We then describe the commonly used level-symmetric and Legendre–Chebyshev (P_n-T_n) quadratures. In the next section, a description of three recently developed quadratures is given: the even–odd moment quadratures, the linear

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discontinuous finite element surface area (LDFESA) quadratures and Icosahedral quadratures. Through a series of reactor physics calculations, we then test the performance of each quadrature set. Calculations are done with the transport codes PENTRAN (Sjoden and Haghighat, 1997) and TITAN (Yi, 2007). We conclude the paper with a discussion of the results.

2. Quadratures on the sphere

The field of numerical integration has a long history and can be traced back to ancient times (Cools, 1997). Indeed the Greek philosophers developed the "Method of Exhaustion" to estimate the area inside of a two-dimensional closed curve. Today we understand the Method of Exhaustion as a technique in numerical integration. Numerical integration (quadrature) remains an active area of research today, with multi-dimensional quadratures of particular importance for three-dimensional radiation transport.

Recall that a quadrature formula is used to approximate a definite integral:

$$I[f] = \int_V f(\mathbf{x}) d^n x \approx \sum_{i=1}^{M} w_i f(\mathbf{x}_i), \tag{4}$$

where $V \subset \mathbb{R}^n$ is the region of integration and $\mathbf{x}_i$ is a quadrature node with associated weight w_i. In developing a quadrature formula, the specific class of functions for which Eq. (4) is to hold must be specified. For example, suppose $V = [-1, 1]$ and we want Eq. (4) to hold for all polynomials of maximum degree $2n-1$. Then we are lead to the Gaussian quadrature

$$\int_{-1}^{1} f(x) dx = \sum_{i=1}^{n} w_i f(x_i), \tag{5}$$

where the nodes x_i are related to the zeros of the nth degree Legendre polynomial and the weights are given by

$$w_i = \frac{2}{(1-x_i)\left[P_n'(x_i)\right]^2}. \tag{6}$$

Note that the dimension of the subspace of polynomials (in one variable) of degree less than or equal to $2n-1$ is $2n$ and, moreover, there are $2n$ degrees of freedom in the quadrature Eq. (4), n nodes and n weights. Thus, Gaussian quadratures are the most efficient in the sense that with $2n$ degrees of freedom, they can integrate $2n$ functions. We remark that this fundamental result is central to showing that the slab-geometry P_n and S_n equations are equivalent (Lewis and Miller, 1993). In contrast, the trapezoidal rule using n nodes can in general integrate up to degree $n-1$ polynomials (Isaacson and Keller, 1966). In the case, the efficiency is $n/2n$ or $1/2$. For slab-geometry, azimuthally-symmetric S_n problems, a number of angular quadratures can be found in (Barros, 1997).

With the goal of discretizing the scattering operator in the Boltzmann transport equation, we now discuss Eq. (4) in the context of $V = \mathbb{S}^2$, the unit sphere in $\mathbb{R}^3$. A natural parametrization of a point $\mathbf{\Omega} \in \mathbb{S}^2$ is

$$\mathbf{\Omega} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^T, \tag{7}$$

where θ is the polar angle and ϕ is the azimuthal angle. We also denote $\mathbf{\Omega} = (\mu, \eta, \xi)^T$, with $\mu = \sin\theta\cos\phi, \eta = \sin\theta\sin\phi$ and $\xi = \cos\theta$. The functions for which we require Eq. (4) to hold will be the spherical harmonics, defined by

$$Y_l^m(\theta,\phi) = (-1)^l \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta) e^{im\phi}, |m| \leqslant l, 0 \leqslant l, \tag{8}$$

where P_l^m is the Associated Legendre Function. In the sequel, we will write $Y_l^m(\theta,\phi) = Y_l^m(\mathbf{\Omega})$. It is a fundamental result, and a key difference between one-dimensional and multi-dimensional transport problems, that Gaussian quadratures *do not* exist in higher dimensions (Reimer, 2003). In fact, this is what prevents the P_n and S_n methods from being equivalent in higher (than one) dimensions. We are thus faced with the task of determining nodes (directions) $\mathbf{\Omega}_i$ and associated weights w_i such that

$$\int_{\mathbb{S}^2} Y_l^m(\mathbf{\Omega}) d\Omega = \sum_{i=1}^{M} w_i Y_l^m(\mathbf{\Omega}_i) \tag{9}$$

holds for as large of degree as possible spherical harmonic.

There are various approaches to developing such a quadrature. One approach, essentially that taken by Carlson and Lee when developing the Level-Symmetric Quadratures (Carlson and Lee, 1961), is to first specify the locations of the nodes $\mathbf{\Omega}_i$ using some type of geometric arguments. Then to determine the weights, one has to solve a linear system of equations derived by enforcing various moment conditions, that is, requiring Eq. (9) to hold for various l and m. A second approach is to take a tensor product of two, one-dimensional quadratures (Longoni and Haghighat, 2001). For example, one can use a Gaussian quadrature in the polar angle and a trapezoidal rule in the azimuthal angle. This approach leads to the so-called Pn-Tn or product quadratures. A third approach is to solve the nonlinear equations formed by writing Eq. (9) for each $0 \leqslant l \leqslant L$ and $|m| \leqslant l$. For a given L, this leads to a system of $(L+1)^2$ nonlinear equations for the $3M$ parameters $(\theta_i, \phi_i, w_i), i = 1, 2, \ldots M$. This approach was taken by Lebedev (Lebedev, 1976) and Ahrens and Beylkin (Ahrens and Beylkin, 2009). To reduce the size of the nonlinear system of equations, a symmetry condition on the location of the nodes can be used. Then a fundamental result of Sobolev (Sobolev, 1962) shows that the number of equations that need to be considered is reduced by a factor of $1/|G|$, where $|G|$ is the size of the symmetry group imposed on the nodes.

In the case of the sphere, a measure of quadrature efficiency is (McLaren, 1963)

$$\eta = \frac{(N+1)^2}{3M}, \tag{10}$$

where N is the maximum degree spherical harmonic the quadrature can integrate and there are M points in the quadrature. Since the subspace of spherical harmonics of maximum degree N contains $(N+1)^2$ linearly independent functions and each of the M quadrature points carries three degrees of freedom, two angles and one weight, we expect η to be close to unity for highly efficient quadratures. In fact, quadratures developed by solving the nonlinear system of equations, Eq. (9), are typically very efficient, with efficiencies of 99% common. In contrast, it can be shown that the product quadratures (e.g. Pn–Tn) are 66% efficient and, through numerical integration, the level symmetric quadratures range in efficiency from 66% to approximately 29% efficient (Ahrens, 2012).

As indicated in Eq. (2), each ordinate in a quadrature set corresponds to an S_n equation. Said differently, if there are M directions in a quadrature set, then one must perform M transport sweeps when inverting the left hand side of Eq. (2). Other considerations aside, for three-dimensional S_n calculations a quadrature with the highest possible efficiency is desirable, since if the scattering moments can be accurately calculated with fewer quadrature points, then there are fewer transport sweeps to be done.

3. Level-symmetric quadrature and Pn–Tn

Level-symmetric (denoted as LS or LQ) quadrature is widely incorporated in lower order quadratures for three-dimensional S_n calculations, and it is often the primary quadrature discussed for