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DISCRETE ORDINATE MAPPING ALGORITHM FOR REGION-BASED QUADRATURE SETS

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ABSTRACT

Frequently in the solution of problems using the discrete ordinates method, it would be convenient to use different quadrature sets in different spatial regions of the problem. For example, when a problem has a highly diffusive region bounding a void region, using a finer quadrature set in the void region would reduce the occurrence of ray effects in the void region. In this paper, we present a method for mapping between quadrature set regions while conserving current on the boundary between regions. We also present an example problem showing that our linear mapping routine accurately captures the streaming of particles between two quadrature set regions, and that the application of flux factors conserves current at the region boundary.

Key Words: Quadrature, Deterministic Transport, Adaptive

1. INTRODUCTION

The neutral particle transport equation is dependent on seven variables: three spatial variables, two angular direction variables, energy, and time. The discrete ordinates method is often applied as a discretization method in the angular variables. Though methods of using different angular discretizations in different energy groups have been devised in the past, traditionally a given angular discretization has been applied globally throughout the entire spatial domain of a problem. However, in many problems it may be advantageous to apply spatial region-based angular discretizations. One example of this is to use a coarser quadrature set in a highly diffusive region and a finer quadrature set in a streaming region. This would reduce ray effects that occur in some transport calculations and increase computational efficiency. A second application of quadrature mapping arises in problems with non-orthogonal reflecting boundaries. In these problems, the quadrature set is not symmetric about the boundary, and quadrature mapping must be performed. In order to avoid errors introduced from mapping between quadrature sets, conservative mapping algorithms must be developed.

In this paper, we explore a basic linear scheme for fairly simple geometries. The goal of our routine is to conserve partial current across a boundary. The particle conservation is a standard requirement to provide consistently reasonable results. Our method provides more accurate results with fewer ordinates and without noticeably increasing the amount of time required to solve the problem.

Three-dimensional quadrature sets have been analyzed for many years. The first quadrature sets proposed were the Level-Symmetric quadrature sets. These had the beneficial property of being rotationally symmetric about all three axes and still being able to integrate lower-order angular polynomials correctly [1]. Another scheme was the product quadrature sets. These sets allow the use of a Gaussian distribution over some range of the polar axis (i.e. polar levels) [2] with an equally-spaced, equally-weighted scheme azimuthally (Chebyshev quadrature) [3]. These schemes are often referred to as Gauss-Chebyshev quadrature sets, Single Gauss-Chebyshev quadrature sets (SGC), or Double Gauss-Chebyshev quadrature sets (DGC). Recently, a widely used quadrature is the Quadruple Range quadrature (QR) developed by Abu-Shumays [4]. This set is also a product quadrature but it ensures accurate integration on an octant basis. This allows for angular flux discontinuities along the axis and results in more accurate results in many problems.

While there have been improvements in quadrature sets, a basic flaw of these discretizations has not been resolved. The fact that the problem must be approximated spatially along a fixed set of specific directions results in ray effects due to fewer directions than needed in some parts of the problem, and computational waste due to more directions than needed in other parts of the problem. To alleviate these two predicaments, the use of different quadrature sets in different spatial regions has been proposed. This work was initially done at Oak Ridge National Laboratory in the mid-1970s in the D/TORT code [5]. They used a simple method for mapping between different quadrature regions. Along a quadrature region boundary, incoming angular flux was passed to the nearest exiting angular flux (as determined by the dot product between the two ordinates). A flux factor was then used to ensure that current density was conserved across the boundary. The method we are proposing builds on Oak Ridge's previous method by applying more exact mapping algorithms.

2. DESCRIPTION OF METHOD

We currently use what we call "linear" mapping. The method uses up to four incoming directions to determine each exiting direction. First, we define the components of the angular direction as:

$$\begin{aligned} \Omega_x &= \mu \equiv \sin\theta\cos\gamma, \\ \Omega_y &= \eta \equiv \sin\theta\sin\gamma, \\ \Omega_z &= \xi \equiv \cos\theta. \end{aligned} \tag{1}$$

The algorithm now proceeds as follows: first, we find the nearest two polar levels with which interpolation is possible. We define the distance between polar levels as

$$d_{pol} = \left|\xi - \xi_{int}\right|. \tag{2}$$

On each of these polar levels, we then determine the nearest two azimuthal directions with which interpolation is possible. We define the distance between azimuthal directions as

$$d_{azi} = \sqrt{\left(\mu - \mu_{int}\right)^2 + \left(\eta - \eta_{int}\right)^2}. \tag{3}$$

For interpolation to be possible there must be a level above and below the interpolated level, and azimuthal points to the left and to the right of the interpolated azimuthal point on each level. We then perform a linear interpolation in μ. If this is not possible (because both points have the same value of μ), linear interpolation is performed in η. If extrapolation is required, a negative flux may be found, which we set to zero. We then determine the total incoming current on the surface and the total outgoing current on the surface. The global flux factor is defined as:

$$f := \frac{\sum_{i=1}^{I} w_i \left(\bar{n} \cdot \bar{\Omega}\right)_i \Psi_i}{\sum_{j=1}^{J} w_j \left(\bar{n} \cdot \bar{\Omega}\right)_j \tilde{\Psi}_j}, \tag{4}$$

where I is the total number of incoming angles and J is the total number of outgoing angles. This factor is then applied to all angular fluxes on the exiting face to globally conserve the current across each face:

$$\Psi_j = f \tilde{\Psi}_j. \tag{5}$$

This method is applied to all faces that lie on the boundary.

3. RESULTS

Initial results were obtained using two sample problems. These problems and their results are discussed in the following sections.

3.1 Two-Cube Test Problem

The test problem is composed of two cubes, one centimeter on each edge, with a 10×10×10 spatial mesh in each cell. The cubes are each separate quadrature regions, and are connected with a mapping boundary. The problem has one energy group and is a purely absorbing medium with a constant isotropic source and vacuum boundary conditions. A diagram is shown in Figure 1.

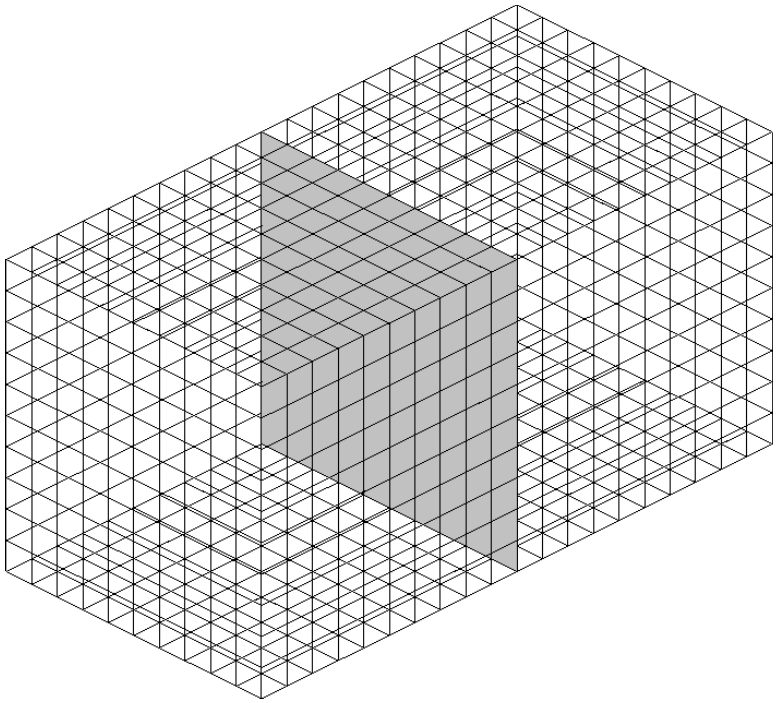


Figure 1. Sample problem geometry.

The quadrature sets used are the SGC quadrature sets, arranged in a triangular pattern similar to the level-symmetric quadrature sets. An example is shown in Figure 2. For this arrangement, with order N, the total number of angles is $N \times (N + 2)$.

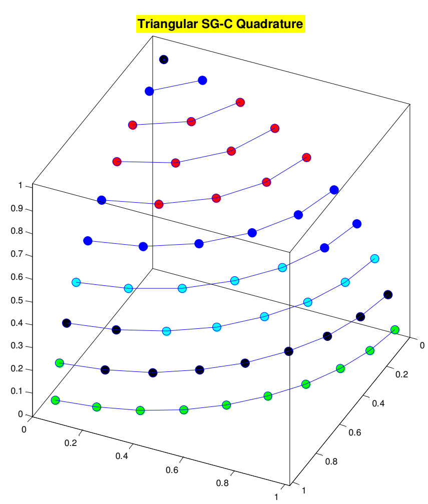


Figure 2. Triangular Single-Gauss Chebyshev Quadrature Set.

For this problem, a finer quadrature set results in a more accurate solution. Figure 3 shows computed scalar flux values for various SGC quadrature orders. The converged volume averaged scalar flux solution for this problem is 0.7499 n/cm^2-s. For the SGC-4 solution (left-most point), there are 48,000 unknowns total, and for the SGC-32 solution (right-most point), there are 2,176,000 unknowns total.

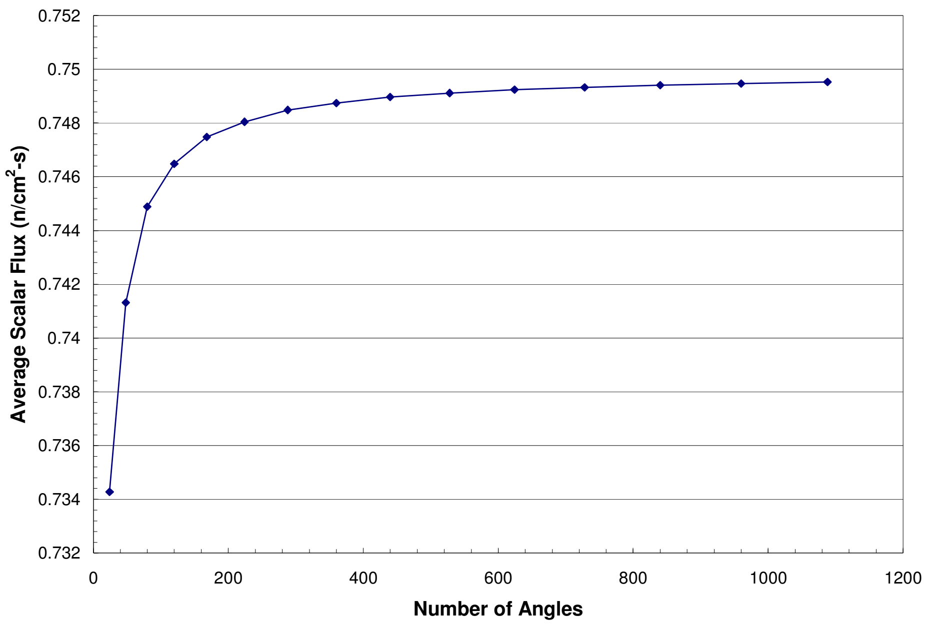


Figure 3. Scalar flux as a function of quadrature order.

The solutions shown in Figure 3 were obtained using the same quadrature set in both regions. Now, we will compare these results with those obtained using a different order SGC quadrature set in each region. The solutions using the following procedure are shown in Figure 4. First, we run the problem with SGC-4 in both regions (48,000 unknowns; shown as the left-most point) and increase the order in the right region to SGC-32 while keeping the left region at SGC-4 (left half of Figure 4). The solution in the left region asymptotes to 0.3680 n/cm^2-s, and the solution in the right region asymptotes to 0.3774 n-cm/s. At this point, there are 1,112,000 unknowns in the problem. The problem-average solution for this case is 0.3727 n/cm^2-s. Next, we increase the quadrature order in the left region to SGC-32. As we do so, both region solutions asymptote to 0.3748 n/cm^2-s. Here there are 2,176,000 unknowns in the problem. Also shown in the plot is the solution using one quadrature region. These results show that, as expected, the scalar flux in the multiple quadrature problem is not as accurate as using the high-order (32) quadrature everywhere, but is more accurate than using the low-order (4) quadrature everywhere.

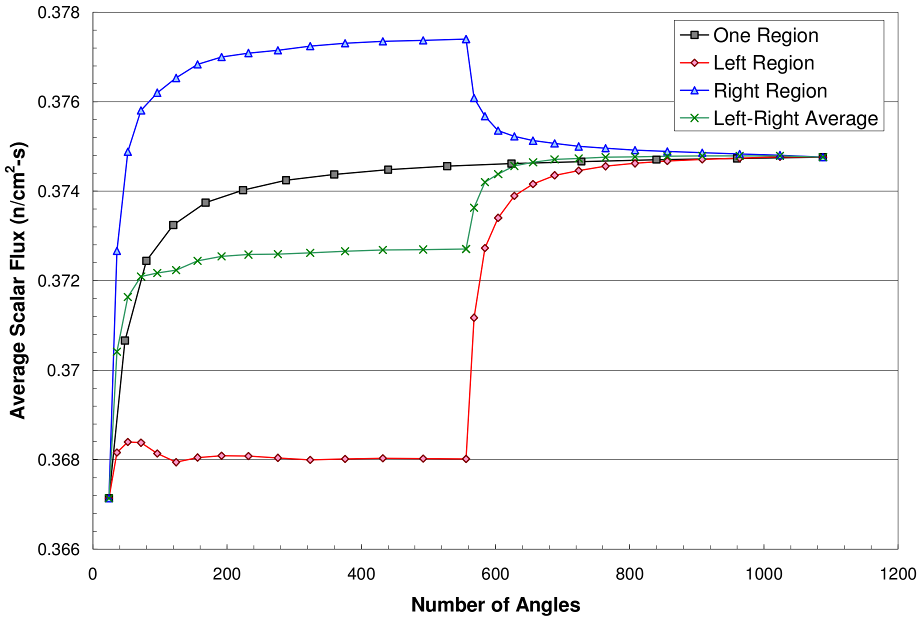
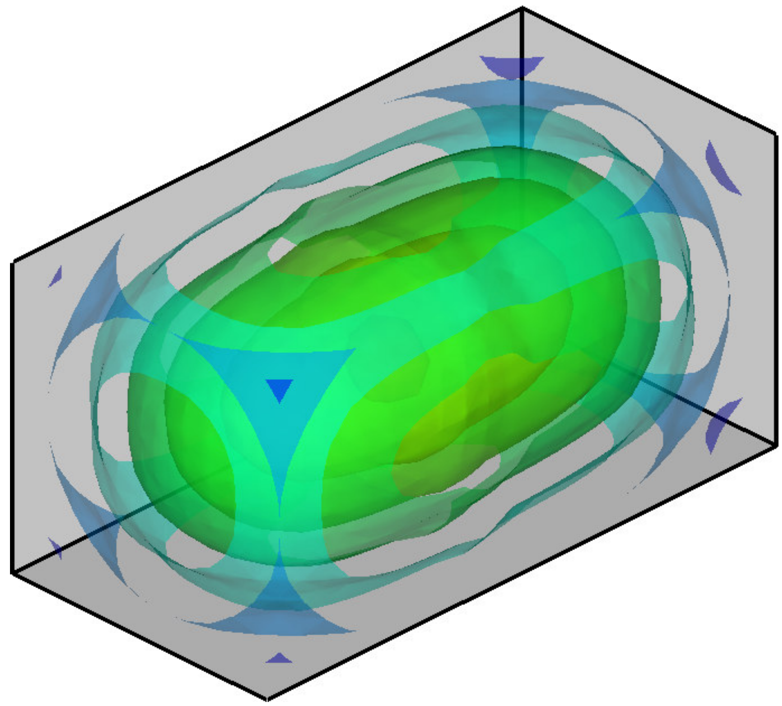
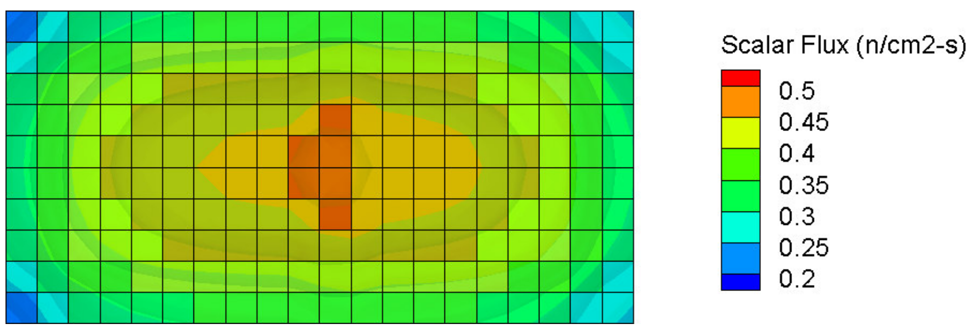


Figure 4. Solutions of example problem using different quadrature set orders in different spatial regions.

In our example, at the center point of the plot, we have reduced the number of angles in the problem by almost a factor of two. The solution at this point is shown in Figure 5. It can be seen in both figures (a) and (b) that there is a discontinuity in the flux at the center boundary. This is a result of the use of linear extrapolation in angle when refining from the low-order quadrature set to the high-order quadrature set. This can be seen by plotting the angular flux along the mapping boundary for a 1D version of this problem. This plot is shown in Figure 6. In this figure, both the S4 solution (square points) and the S16 solution (round points) are shown along with the analytic solution at this spatial location. One can see that the scalar flux resulting from the S16 points will be higher than the scalar flux resulting from the S4 points. This results in a small (~4.76%) discontinuity in scalar flux, which is shown in Figure 7, where the black line is the analytic in space and angle solution and the green line is the analytic in space, but discrete ordinates in angle, solution. This discontinuity is more pronounced in the spatially discretized solution shown in Figure 5. The remedy to this discontinuity in both flux and current will be researched and presented in subsequent papers.



(a)



(b)

Figure 5. Scalar flux in the test problem; (a) is a 3D isosurface plot, and (b) is a 2D slice through the center of the problem. The S4 region is on the left and the S32 region is on the right of the figures.

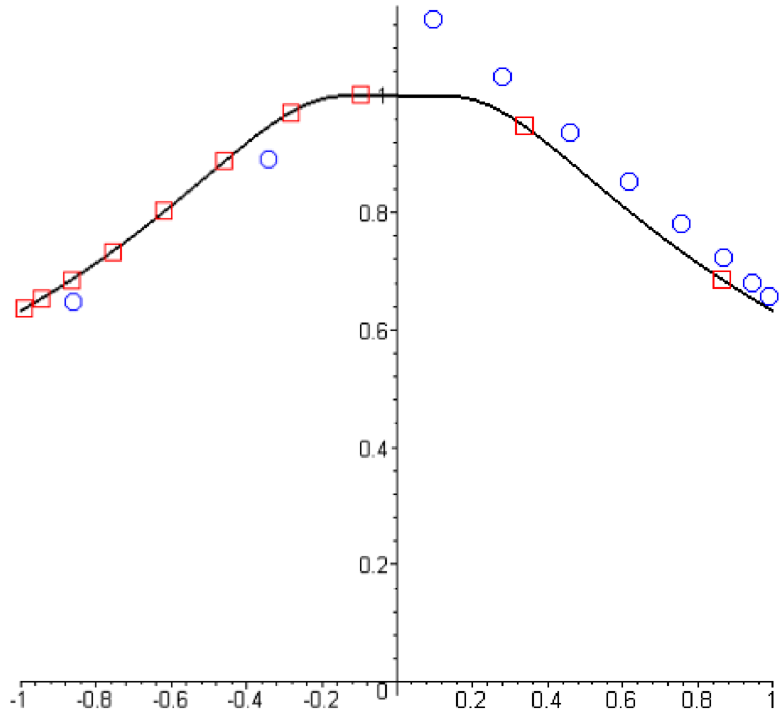


Figure 6. Angular flux at center point of the test problem.

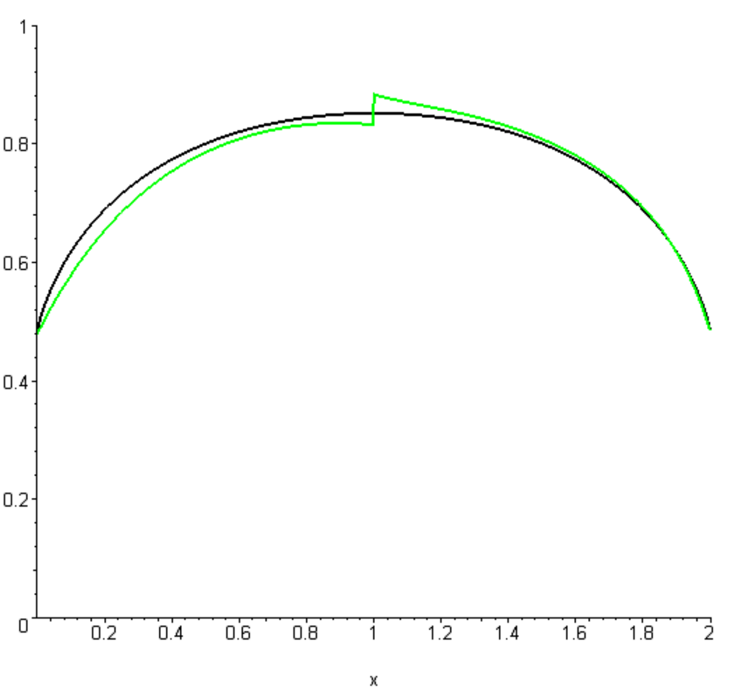


Figure 7. Scalar flux in 1D version of the test problem.

4. CONCLUSIONS

We have shown that our linear mapping routine accurately captures the streaming of particles between quadrature set regions, and that the application of flux factors conserves current at the boundary of the regions. While these results are encouraging, in future papers we will examine what effect on solution accuracy is provided by more accurate, higher order mapping algorithms, and will include consideration of more difficult problems.

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REFERENCES

1. E. E. Lewis and W. F. Miller, Jr., *Computational Methods of Neutron Transport,* American Nuclear Society, La Grange Park, Illinois, USA (1993).
2. A. H. Stroud and D. Secrest, *Gaussian Quadrature Formulas*, Englewood Cliffs, NJ: Prentice-Hall (1966).
3. P. Tchebicheff, "Sur les quadrature sets." J. de. Math. Pures appliq. **19**, 19 (1874).
4. I. K. Abu-Shumays, "Compatible Product Angular Quadrature for Neutron Transport in x-y Geometry," *Nucl. Sci. Eng.,* **64**, 299 (1977).
5. W. W. Engle, F. R. Mynatt, M. B. Emmett, and M. L. Williams, "A Summary of the ORNL Shield Design Supporting Analysis for the FFTF," *Fifth International Conference on Reactor Shielding, Knoxville, TN, April 18-22, 1977; Proceedings,* pp. 44-53 (1977).