M&C 2001 Salt Lake City, Utah, USA, September 2001.

DEVELOPMENT OF NEW QUADRATURE SETS WITH THE "ORDINATE SPLITTING" TECHNIQUE

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Keywords: quadrature set, ordinate splitting, Legendre polynomials, Chebyshev polynomials

ABSTRACT

The Discrete Ordinate Method (S_N) is one of the most widely used techniques to solve the linear Boltzmann equation. A commonly used technique for the generation of discrete ordinates and associated weights (quadrature set) is the level-symmetric. However, this technique is limited to order S_{20}. To deal with highly angular dependent situations, we have developed different quadrature techniques including P_N-EW, P_N-T_N and a new angular refinement approach referred to as "ordinate splitting". We have tested these new quadrature sets using the Kobayashi 3-D problem 3, and demonstrated that P_N-T_N with ordinate splitting is an effective approach for highly directional problems.

1. INTRODUCTION

The discrete ordinate method is used to solve the neutron transport equation. The angular variable $\hat{\Omega}$, in the transport equation, is discretized in a finite number of directions and the angular flux is evaluated only along these directions. Each discrete direction can be visualized as a point on the surface of a unit sphere with which a surface area, denoted as weight, is associated[1].

A major issue affecting the accuracy of the S_N method is selecting an appropriate set of directions. In order to preserve the physics, the general criteria for generating quadrature sets, are preserving symmetry and the moments of the direction cosines.

In the level-symmetric quadrature set (LQ_N)[1], the discrete directions are chosen to be fully symmetric with respect to all coordinate axes. There is a total of N(N+2) directions on the unit sphere, where N is the S_N order. The weight associated to each direction is evaluated by satisfying the moment conditions for direction cosines. The LQ_N technique, however, is limited to order 20, because beyond which some of the weights become negative.

In order to prevent this difficulty, B.G. Carlson proposed[2] the Equal Weight Quadrature set (EQ_N), which is characterized by positive weights for any S_N order. In the EQ_N technique, all the direction weights are set equal to $w = 1/[N(N+2)]$.

Other quadrature sets have been derived, by relaxing the constraints imposed by the LQ_N method[3]. For this purpose, the Gauss quadrature technique has been used to derive quadrature sets based on the Legendre and Chebyshev polynomials, which yield positive weights[1,4]. In a recent study[5], two new quadrature sets (UE_N and UG_N) have been derived. The UE_N quadrature set is derived by uniformly partitioning the unit sphere in the number of direction defined by the S_N order. The UG_N quadrature set selects the ordinates along the z-axis as roots of Legendre polynomials.

In this paper we present different approaches for generating sets of discrete directions, including standard LQ_N, Legendre Equal-Weight (P_N-EW), Legendre-Chebyshev (P_N-T_N) and a new biasing technique referred to as the “ordinate splitting”. We use the conventional ordering of LQ_N. The advantage of P_N-EW and P_N-T_N over LQ_N is the ability of generating quadrature sets beyond order 20.

This paper is organized as follows. In section 2, we discuss the LQ_N quadrature set. In section 3, we discuss the P_N-EW quadrature set. Section 4 discusses the P_N-T_N quadrature set. In section 5 we verify the even moment condition for P_N-EW and P_N-T_N quadrature sets. Section 6 describes the Ordinate Splitting Technique. Section 7 examines the effectiveness of these new quadrature sets using the Kobayashi[6] benchmark problem 3.

2. DISCUSSION ON THE LEVEL-SYMMETRIC QUADRATURE (LQ_N) SET

In the LQ_N method, directions are selected based on the following formulation[1]:

$$\mu_i^2 = \mu_1^2 + (i-1)\Delta \quad \text{where } \Delta = \frac{2(1-3\mu_1^2)}{(N-2)} \text{ and } 2 \le i \le \frac{N}{2} \;;\; 0 < \mu_1^2 \le \frac{1}{3} \qquad (1)$$

This formulation is derived, by considering $\mu_i^2 + \eta_j^2 + \xi_k^2 = 1$ and $i + j + k = \frac{N}{2} + 2$, where N refers to the number of levels and i,j,k are indeces for direction cosines.

In Eq. 1 the choice of μ_1 determines the distribution of directions on the octant. If the value of μ_1 is small, the ordinates will be clustered near the poles of the sphere; on the opposite, if the value of μ_1 is large, the ordinates will be placed far from the poles[3].

To obtain the weights associated with directions, LQ_N uses moment conditions of the direction cosines as follows[7]:

$$\sum_{i=1}^{M} w_i = 1.0 \qquad (2)$$

$$\sum_{i=1}^{M} w_i \mu_i^n = \sum_{i=1}^{M} w_i \eta_i^n = \sum_{i=1}^{M} w_i \xi_i^n = 0.0 \quad \text{for n odd} \tag{3}$$

$$\sum_{i=1}^{M} w_i \mu_i^n = \sum_{i=1}^{M} w_i \eta_i^n = \sum_{i=1}^{M} w_i \xi_i^n = \frac{1}{n+1} \quad \text{for n even} \tag{4}$$

Here, Eq. 2 is a normalization condition for the weights. Eqs. 3 and 4 respectively represent the *odd-moment* and *even-moment* conditions. The odd-moment condition is implicitly satisfied because the quadrature set must be symmetric over the unit sphere, and it should be invariant with respect to 90-degree axis rotation. Eq. 4 represents the even-moment conditions required in order to properly integrate the Legendre polynomials[7]. It is worth noting that using the level-symmetric technique, for N levels, the total number of directions is M=N(N+2). The weight associated to each direction, called point weight, is then evaluated with another set of equations. For example, the case of a S_8 LQ_N set, this condition can be formulated as follows:

$$2p_1 + 2p_2 = w_1;\ 2p_2 + p_3 = w_2;\ 2p_2 = w_3;\ 1p_1 = w_4, \tag{5}$$

where p_1, p_2 and p_3 are point weights associated to each direction, and w_1, w_2, w_3, w_4 are the weights associated to the levels, as shown in Fig. 1. Eq. 5 presents the point weight distribution for each direction.

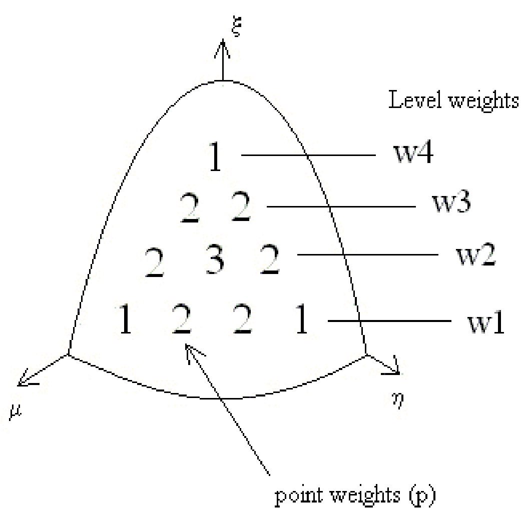


Fig. 1 Point weight arrangement for a S_8 LQ_N quadrature set

Beyond the order S_{20}, Eqs. 2 to 4 yield unphysical negative weights. As an example, in Fig. 2, we present the directions selected by the S_{16} LQ_N method in one octant.

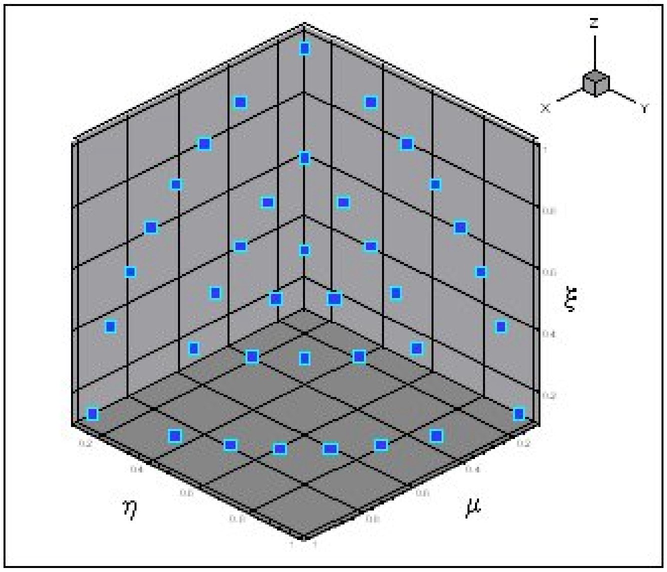


Fig. 2 Discrete directions selected on one octant with S_{16} LQ_N quadrature set

3. LEGENDRE EQUAL-WEIGHT (P_N-EW) QUADRATURE SET

In order to develop a quadrature set which is not limited to order S_{20}, we have investigated the Gauss-Legendre quadrature technique[1,4]. In this quadrature set we utilize the same arrangement of directions as the LQ_N, but the directions and weights are evaluated differently. Given the S_N order for the discrete set of directions, we obtain the Legendre polynomials applying the following recursive formulation[8]:

$$(j+1)P_{j+1} = (2j+1)\xi P_j - jP_{j-1} \qquad \text{for j = 0…N} \tag{6}$$

$$-1 < \xi < 1 \quad P_{-1}(\xi) = 0 \quad P_0(\xi) = 1$$

The ordinates, i.e. ξ, along the z-axis are the roots of the Legendre polynomials given by Eq. 6. Once we have evaluated the ordinates along z-axis we obtain the weights associated to each level with the following recursive formula[8]:

$$w_i = \frac{2}{(1-\xi_i^2)\left[\left(\frac{dP_N}{d\xi}\right)_{\xi_i}\right]^2} \ , \quad i = 1 \ldots \frac{N}{2} \tag{7}$$

And the weight associated with each direction is given by:

$$p_{i,j} = \frac{w_i}{j} \quad \text{for } i = 1 \ldots \frac{N}{2} \tag{8}$$

where $j = 1 \ldots \frac{N}{2} - i + 1$ is the number of directions with equal weights on the i^{th} level.

In order to evaluate the azimuthal angle on each level, we equally divide a 90 degrees angle by the number of angular intervals (i.e., $\frac{N}{2} - i + 2$) between directions.

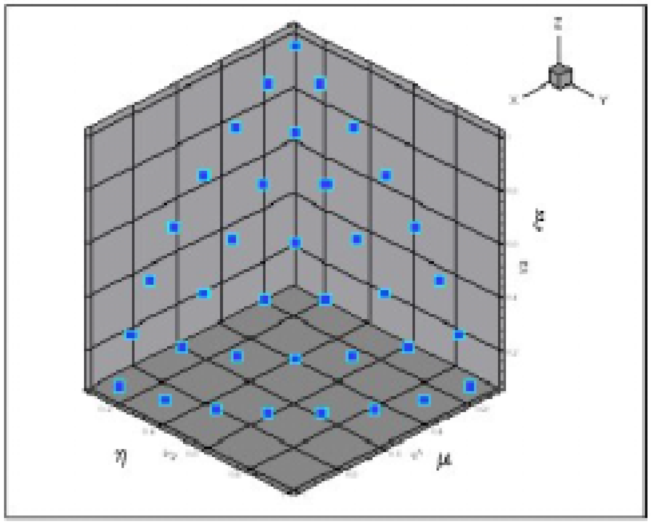


Fig. 3 Discrete directions selected on one octant with S_{16} P_N-EW quadrature set

In Fig. 3, we show the directions selected by P_N-EW technique for a quadrature set of order S_{16}.

4. LEGENDRE-CHEBYSHEV (P_N-T_N) QUADRATURE SET

In the P_N-T_N methodology, similar to P_N-EW, we set the ξ levels on the z-axis equal to the roots of Legendre polynomials, but for the azimuthal angles on each level we use the roots of the Chebyshev T_N polynomials of first kind[4]. The Chebyshev polynomials of first kind have the following formulation:

$$T_l[\cos(\omega)] \equiv \cos(l\omega) \tag{9}$$

The Chebyshev polynomials are orthogonal and satisfy the following condition:

$$\int_{-1}^{1} dy T_l(y) T_k(y)(1-y^2)^{-1/2} = \begin{cases} 0, l \neq k \\ \pi, l = k = 0 \\ \pi/2, l = k \neq 0 \end{cases} \tag{10}$$

$$y = \cos(\omega)$$

Again, using the ordering of the LQ_N quadrature set, we set the azimuthal angles on each level using the following formulation[4]:

$$\omega_{l,i} = \left(\frac{2l-2i+1}{2l}\right)\frac{\pi}{2} \qquad \omega_{l,i} \in \left(0, \frac{\pi}{2}\right), \; i = 1 \ldots l \tag{11}$$

In Eq. 11, *l* is the level number. The level and point weights are generated in the same way as for the P_N-EW. Both P_N-EW and P_N-T_N sets do not present negative weights for S_N orders higher than 20.

5. VERIFICATION OF THE EVEN-MOMENT CONDITION FOR P_N-EW AND P_N-T_N METHODS

The main advantage of the LQ_N technique is the fact that it preserves moments of the direction cosines, thereby leading to an accurate solution. In this section, we compare the new quadrature sets based on the magnitude of the even moments of the direction cosines. Table 1 gives the moments for the P_N-EW. As expected, P_N-EW yields accurate moments along the z-axis, while its azimuthal direction cosines deviate from the expected values by as much as ~17 %.

Table 1 Even-Moments for P_N-EW S_{30} set

Moment Order (n even)	$\sum_{i=1}^{M} w_i \mu_i^n$	$\sum_{i=1}^{M} w_i \eta_i^n$	$\sum_{i=1}^{M} w_i \xi_i^n$	$\frac{1}{1+n}$
2	0.333333333	0.333333333	0.333333333	0.333333333
4	0.194318587	0.194318587	0.2	0.2
6	0.135907964	0.135907964	0.142857143	0.142857143
8	0.103874123	0.103874123	0.111111111	0.111111111
10	0.083691837	0.083691837	0.090909091	0.090909091
12	0.06983611	0.06983611	0.076923077	0.076923077
14	0.059749561	0.059749561	0.066666667	0.066666667
16	0.052087133	0.052087133	0.058823529	0.058823529
18	0.046074419	0.046074419	0.052631579	0.052631579
20	0.041234348	0.041234348	0.047619048	0.047619048
22	0.037257143	0.037257143	0.043478261	0.043478261
24	0.033932989	0.033932989	0.043478261	0.043478261
26	0.031114781	0.031114781	0.037037037	0.037037037
28	0.028696358	0.028696358	0.034482759	0.034482759
30	0.026599209	0.026599209	0.032258065	0.032258065

It is clear from Table 2 that the P_N-T_N quadrature set completely satisfies the even-moment condition. This is possible because both roots of Legendre and Chebyshev polynomials satisfy the even-moment condition given by Eq. 4. Fig. 4 shows the directions selected by the P_N-T_N technique for a S_{30} order.

Table 2 Even-Moments for P_N-T_N S_{30} set

Moment Order (n even)	$\sum_{i=1}^{M} w_i \mu_i^n$	$\sum_{i=1}^{M} w_i \eta_i^n$	$\sum_{i=1}^{M} w_i \xi_i^n$	$\frac{1}{1+n}$
2	0.333333333	0.333333333	0.333333333	0.333333333
4	0.199999962	0.199999962	0.2	0.2
6	0.142857143	0.142857143	0.142857143	0.142857143
8	0.111111111	0.111111111	0.111111111	0.111111111
10	0.090909091	0.090909091	0.090909091	0.090909091
12	0.076923077	0.076923077	0.076923077	0.076923077
14	0.066666667	0.066666667	0.066666667	0.066666667
16	0.058823529	0.058823529	0.058823529	0.058823529
18	0.052631579	0.052631579	0.052631579	0.052631579
20	0.047619048	0.047619048	0.047619048	0.047619048
22	0.043478261	0.043478261	0.043478261	0.043478261
24	0.043478261	0.043478261	0.043478261	0.043478261
26	0.037037037	0.037037037	0.037037037	0.037037037
28	0.034482759	0.034482759	0.034482759	0.034482759
30	0.032258065	0.032258065	0.032258065	0.032258065

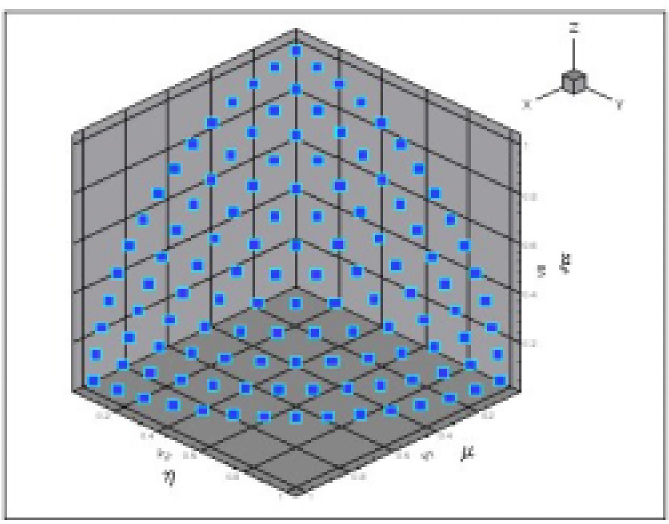


Fig. 4 Discrete directions selected on one octant with S_{30} P_N-T_N quadrature set

6. THE ORDINATE SPLITTING TECHNIQUE

The Ordinate Splitting Technique is developed for solving problems with highly peaked angular flux and/or source. The idea is to introduce more directions at local regions; for this purpose we split a direction into a number of directions with equal weights. These directions are positioned symmetrically around the direction of interest and their weights are calculated by equally dividing the original weight among the new split directions and the direction of interest. This technique because of its local refinement can be considered as a biasing approach.

Currently we divide the solid angle, associated to the direction of interest, into equal size sectors. Then we place the directions on the corner and on the midpoint of the side of the sectors, while the original direction is at the center as shown in Fig. 5. A proper selection of the sector surrounding the original direction is performed to avoid overlapping with other directions. The number of additional directions is chosen with a parameter called segmentation in the following way:

$$\#directions = (2 * nseg - 1)^2 \quad (12)$$

Fig. 6 shows a S_{16} P_N-T_N quadrature set with three split angles; for this case we have set nseg = 2.

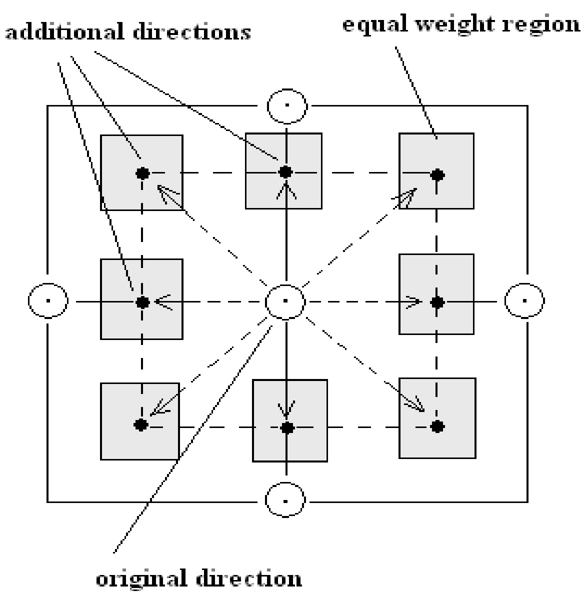


Fig. 5 Ordinate Splitting Technique

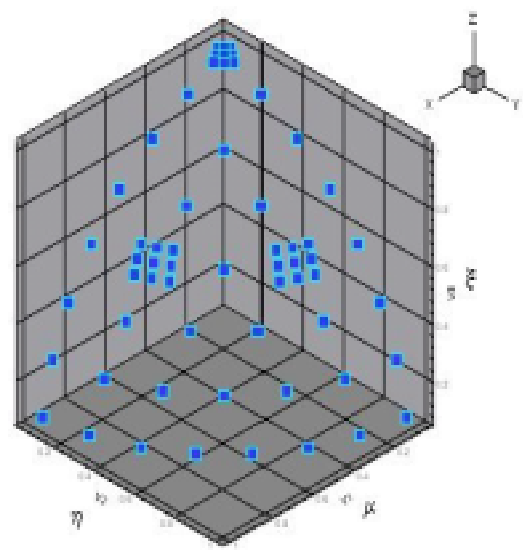


Fig. 6 S_{16} P_N-T_N quadrature set modified with Ordinate Splitting Technique

7. RESULTS

We have implemented the P_N-EW and P_N-T_N techniques with the ordinate splitting approach into the PENTRAN 3-D parallel code[7]. We have also enabled the LQ_N set to use the ordinate splitting technique. To examine the effectiveness of the new quadrature sets, we have used the first axial slice of the Kobayashi 3-D benchmark problem 3 with pure absorber[6]. In Fig. 7, we show two mesh distributions, Fig. 7a is obtained from our previous study[9] in which we selected an appropriate variable mesh; Fig. 7b shows a uniform mesh distribution that we have developed for the current study. The uniform mesh is used in order to be able to identify the effect of angular quadrature type and order. The reference analytical solutions are evaluated at two spatial zones shown in Figs. 7a and 7b (zone 1 ≡ along y-axis, at every 10 cm intervals between 5 and 95 cm; zone 2 ≡ along x-axis, y = 55 cm, every 10 cm, between 5 cm and 55 cm).

The computational resource utilized for running the tests is the PSTTG[1] PCTRAN Cluster, with a 600 MHz Intel Pentium-III processor and 1 GB RAM memory for each node

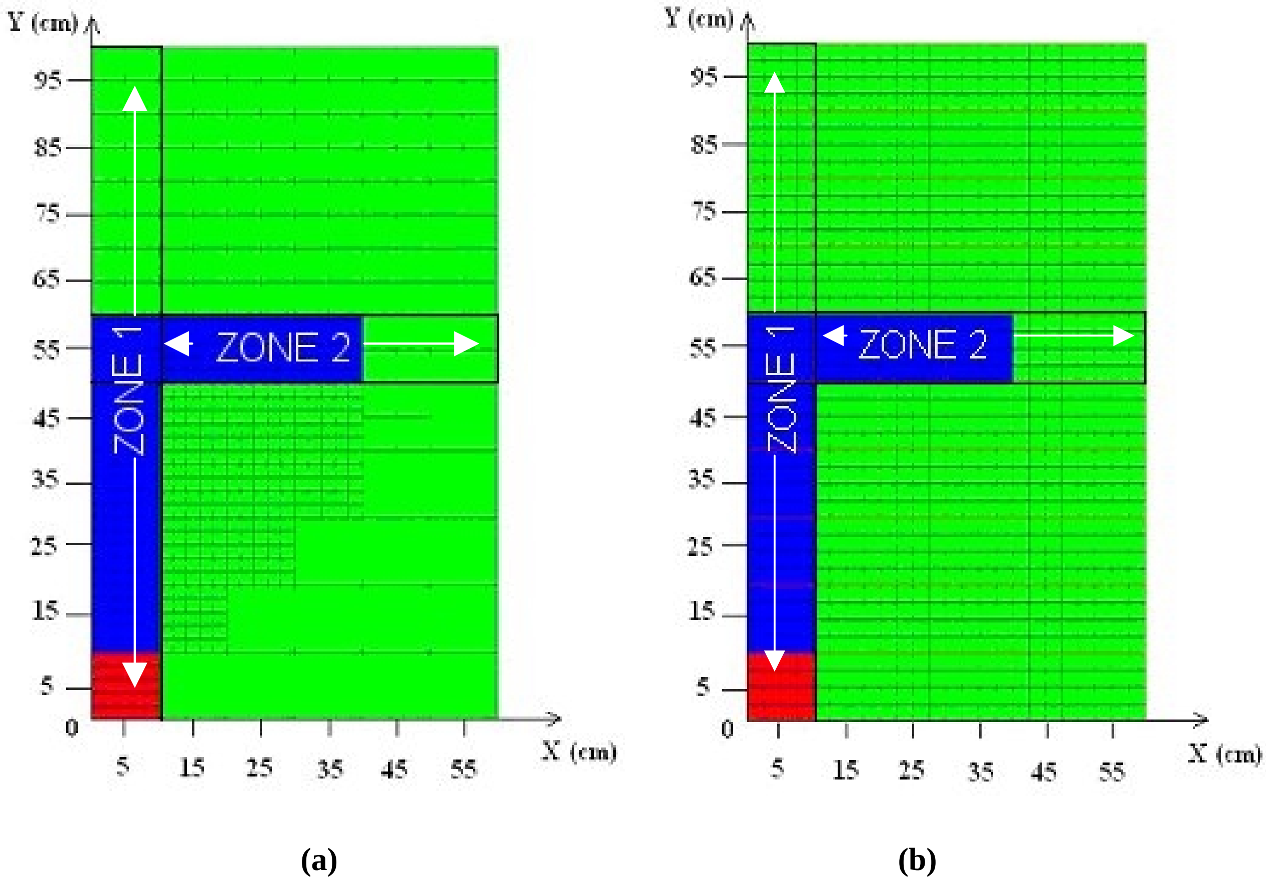


Fig. 7 Mesh distribution for the Kobayashi 3-D problem 3 (first axial slice)

In Fig. 8, we show the ratio of analytical and numerical solutions for the LQ_N, P_N-EW and P_N-T_N schemes of order 20 for zone 1. In this figure, we have also shown our previous solution, which uses variable meshing of Fig. 7a. In the previous solution, by taking advantage of the variable meshing, the LQ_N set yields a maximum error of ~6% in zone 1, and ~9% in zone 2. In the current study, the LQ_N set with uniform spatial mesh

[1] Penn State Transport Theory Group

yields a maximum relative error of ~10% in zone 1 and ~22% in zone 2. We can observe in Fig. 8 that P_N-EW set underestimates (<40%) the flux, because this set has fewer directions near the y-axis as compared to the P_N-T_N and LQ_N sets.

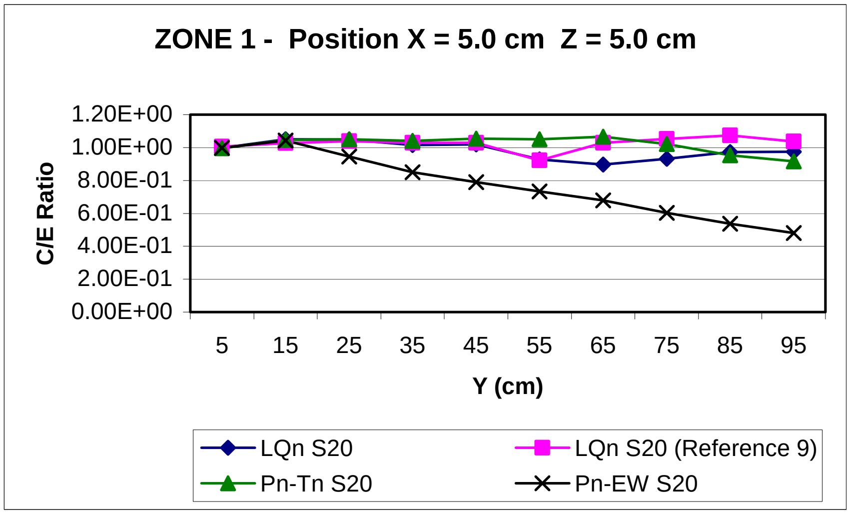


Fig. 8 Comparison of S_{20} quadrature sets at Zone 1

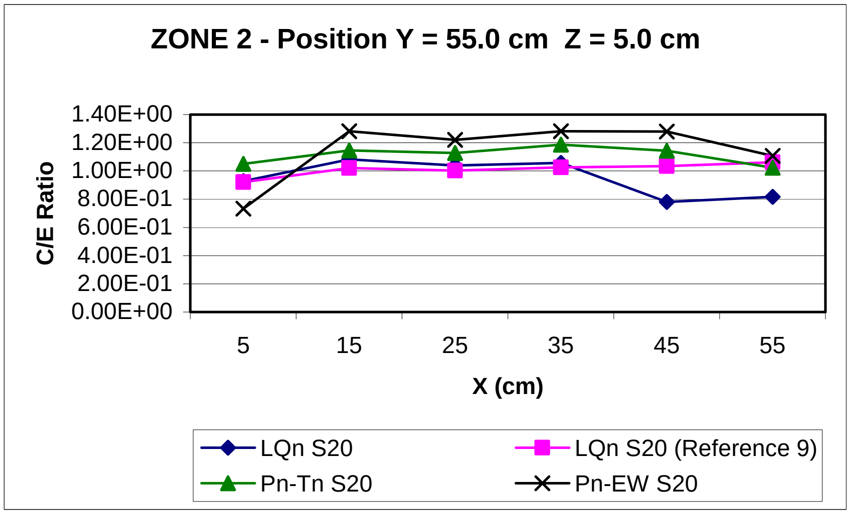


Fig. 9 Comparison of S_{20} quadrature sets at Zone 2

In Fig. 9, we show the comparison in zone 2 of the benchmark problem. The P_N-T_N quadrature set generates results comparable to LQ_N. The maximum relative error for P_N-T_N is ~19%, while for LQ_N it is ~22%. The P_N-EW generates an error of about 52% due to the reason explained earlier.

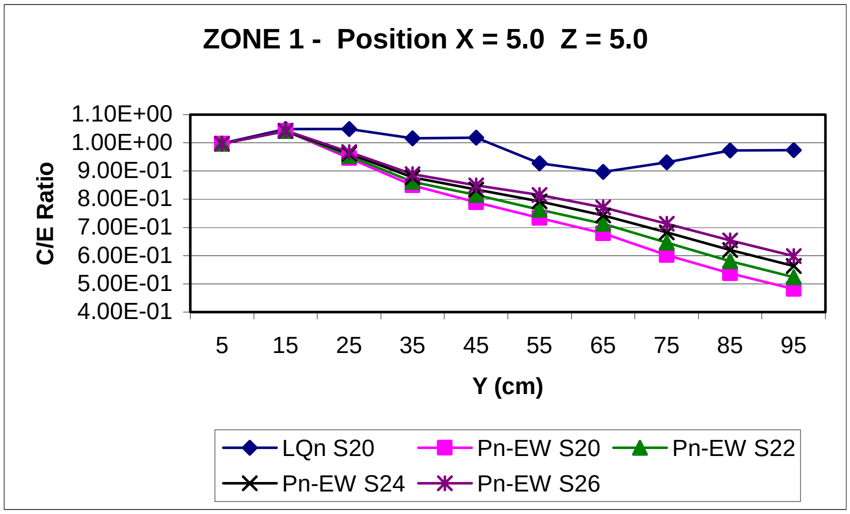


Fig. 10 Comparison of P_N-EW quadrature sets for different orders at Zone 1

In Figs. 10 and 11, we show the results obtained with P_N-EW set of different orders as compared to S_{20} LQ_N. As we can see in zone 1 (Fig. 10), the P_N-EW is not as accurate as LQ_N, because the directions are not clustered near the y-axis. Here the solution somewhat improves by increasing the S_N order. As shown in Fig. 11, in zone 2, the P_N-EW set yields inaccurate results, with a maximum relative error of ~36% for the S_{20} case.

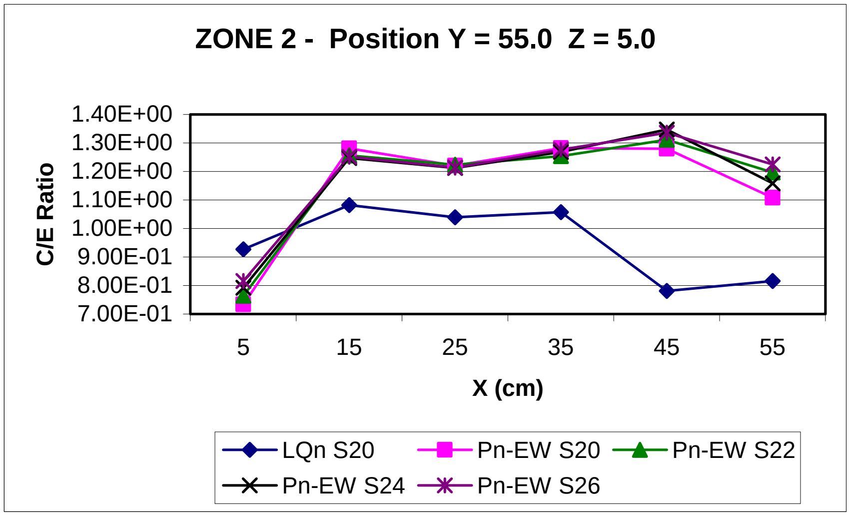


Fig. 11 Comparison of P_N-EW quadrature sets for different orders at Zone 2

In Fig. 12, we compare the P_N-T_N set of orders S_{20}, $S_{22,}$ S_{24} and S_{26} with the S_{20} LQ_N. It appears that the increase in the quadrature order does not have a noticeable effect. This can be attributed to the fact we have kept the same spatial mesh.

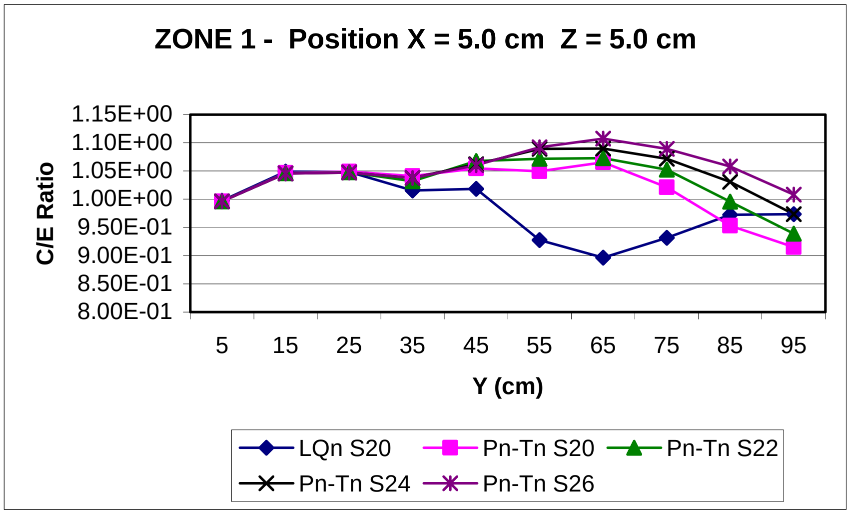


Fig. 12 Comparison of P_N-T_N quadrature sets for different orders at Zone 1

In zone 2 (Fig. 13), we can observe that S_{22} P_N-T_N is more accurate than LQ_N set. The S_{22} P_N-T_N yields a maximum relative error of ~9% compared to ~22% from LQ_N. Again, in zone 2, the accuracy somewhat decreases as the S_N order increases, because the spatial mesh is kept constant.

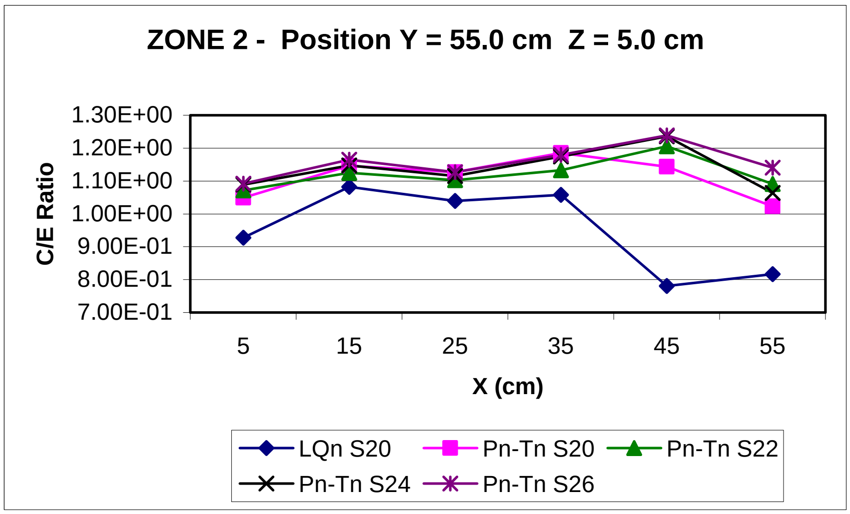
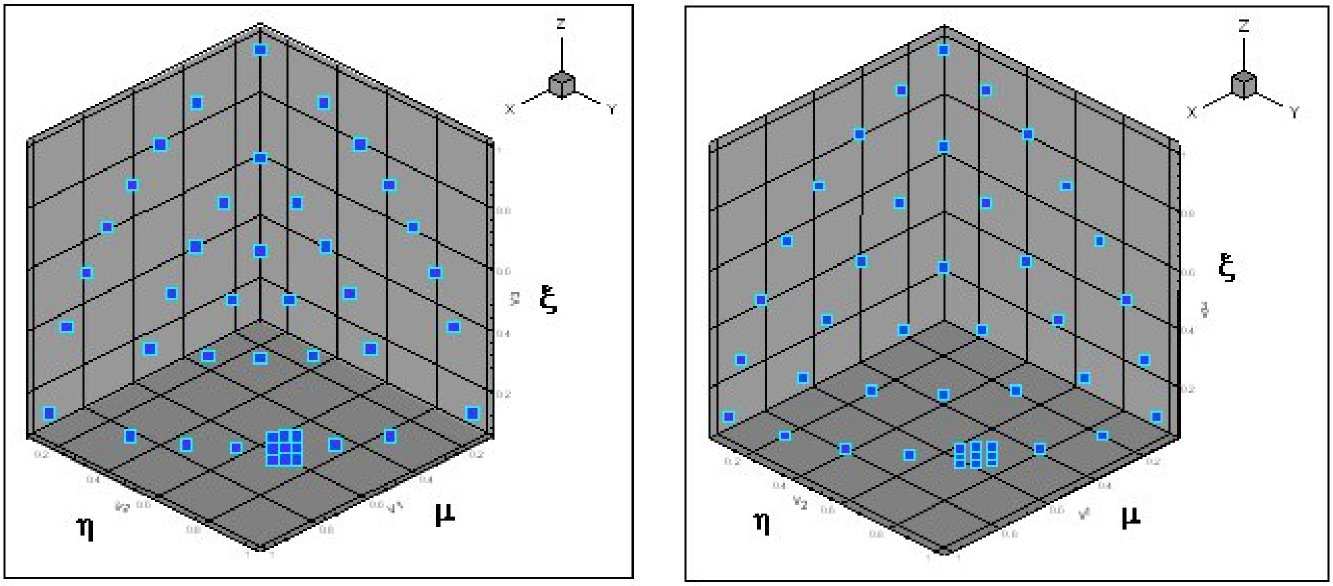


Fig. 13 Comparison of P_N-T_N quadrature sets for different orders at Zone 2

Figs. 15-16 show the effect of ordinate splitting technique. For both LQ_N and P_N-T_N quadrature sets of order 16, we have split direction 33 into 9 directions as shown in Figs. 14a and 14b. The S_{16} P_N-T_N set yields accurate results with a maximum relative error of ~13%, while the S_{16} LQ_N yields a maximum relative error of ~16%.



(a) **(b)**

Fig. 14 Ordinate Splitting Technique applied to S_{16} LQ_N and S_{16} P_N-T_N on direction 33 with segmentation equal to 2.

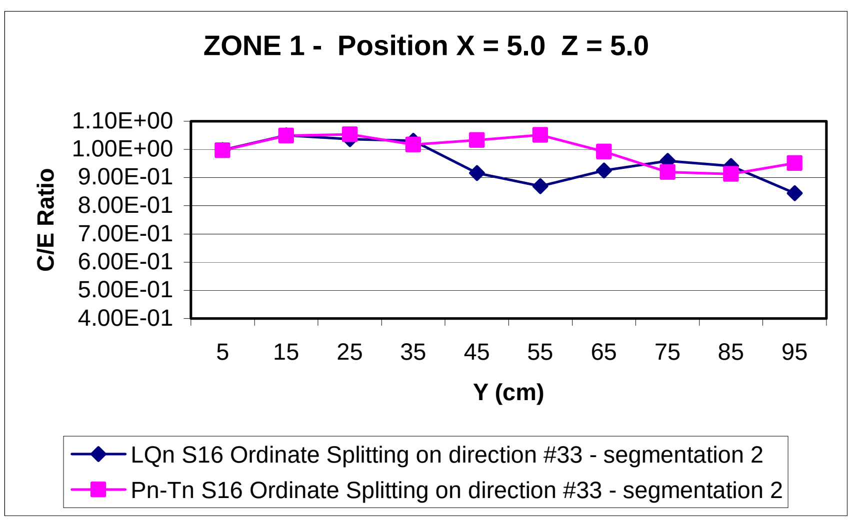


Fig. 15 Ordinate Splitting Technique applied to S_{16} LQ_N and S_{16} P_N-T_N at Zone 1

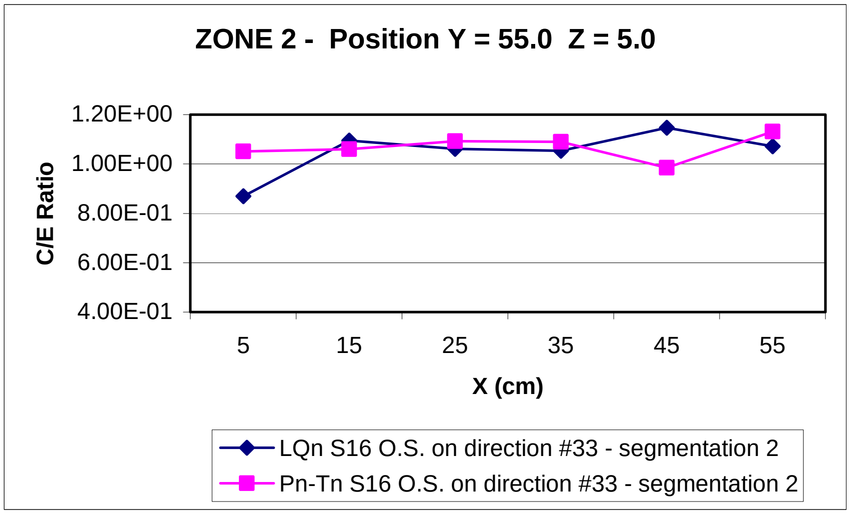


Fig. 16 Ordinate Splitting Technique applied to S_{16} LQ_N and S_{16} P_N-T_N at Zone 2

By comparing these results with those obtained in the previous cases, we notice that a low order quadrature set like S_{16} P_N-T_N, modified with the ordinate splitting technique, can yield more accurate results than a high order standard quadrature set like S_{20} LQ_N. The S_{16} P_N-T_N set, with ordinate splitting, yields a maximum relative error equal to ~13%, while the standard S_{20} LQ_N yields an error equal to ~22%. By using the ordinate splitting technique we can also reduce the computational cost, by reducing the total number of discrete directions utilized. S_{20} LQ_N has a total of 440 directions, while the S_{16} P_N-T_N, refined with the ordinate splitting technique, uses 313 directions. This reduction in the number of directions results in ~20% reduction in the computational time.

CONCLUSIONS

We have developed and tested different quadrature sets based on the P_N-EW and P_N-T_N techniques and a new approach of "ordinate splitting". The quadrature sets that we derived are not limited by negative weights. It is demonstrated that P_N-T_N quadrature set preserves the integrals of the directions cosine similar to the level-symmetric technique. Moreover, the use of the "ordinate splitting" technique is very effective for solving problems with highly directional source and flux. This technique has resulted in accurate results while reducing the computational cost.

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