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TITLE: [illegible]

LA-UR--87-3621

DE88 001803

AUTHOR(S): [illegible]

SUBMITTED TO: [illegible] Computational Methods in High Temperature Physics [illegible] Meeting, held February [illegible]

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Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

USE OF THE CHEBYSHEV-LEGENDRE QUADRATURE SET
IN DISCRETE - ORDINATE CODES

by

Wallace F. Walters

Radiation Transport Group, X-6
LOS Alamos National Laboratory
Los Alamos. New Mexico 87545

ABSTRACT

The Chebyshev--Legendre (G-L) quadrature set has been implemented in the neutron transport section of the TWODANT code. The C-L quadrature set has two advantages as compared to other quadrature sets. First, it is possible to easily generate S_N orders up to S_{100} with weights that are positive. TWODANT has been used to carry out, calculations with as many as **10,000** discrete directions with the C-L quadrature set. Second, a product C-L set or order N will integrate *exactly* all the terms in the scattering source arising from P_{N-1} scattering. For example, the S_4 set. will correctly integrate all scattering source terms if a P_3 scattering approximation is used. In TWODANT, users normally use the current S_8 quadrature set in the belief that, P_3 scattering will be treated correctly. The S_8 set consists of some 40 directions and many times results in problem models that require excessive computer memory. The C-L S_4 set integrates exactly all the source terms associated with a P_3 expansion and consists of only **16** discrete directions. The results of test calculations, using both the current set and the C-L set in TWODANT, indicate that when high-order scattering is not significant, the two sets give answers that, are in good agreement.

I. INTRODUCTION

Despite all the work that has been published on discrete ordinate quadrature sets, the criteria used to judge if one set is "better" than another has never been unambiguously established. In this paper, the requirement that. the quadrature be capable of integrating the greatest number of spherical harmonics and products of spherical harmonics will be shown to be critically important for the exact. treatment. of forward peaked anisotropic scattering. This type of scattering occurs for fast. neutrons and for gamma- ray photons. The Chebyshev-Legendre quadrature set. examined in Refs. I and 2 will be shown to be efficient for the integration of the spherical harmonics; and hence, the quadrature set of choice for highly anisotropic scattering. Two simple sample problems exhibiting forward peaked scattering are examined. The results obtained from these sample calculations point out clearly the need for this type of quadrature set for this class of problem. A third test. problem, a uranium cylinder. is studied and it is found that the new quadrature set is superior for this simplc problem also, This quadrature set has been implemented in the unclassified code TWODANT.[3]

II. BACKGROUND

The coordinate system used in this discussion is indicated in Fig. 1. This is the system for a cylindrical problem. In x-y geometry, η is the y-direction cosine, μ is the x-direction cosine, and ξ is the z-direction cosine.

If the scattering transfer probability is assumed to be reprcscntcd by a finite Legendre polynomial expansion

$$\sigma_s\left(E' \to E\right) = \sum_{n=0}^{N} \frac{2n+1}{4\pi} P_n\left(\mu_0\right)\sigma_{sn}\left(E' \to E\right) \quad .$$

The multigroup-transport. equation becomes

$$\nabla \cdot \left(\Omega\psi_g\right) + \sigma_{tg}\psi_g = \sum_{h=1}^{G}\sum_{n=0}^{N}\left(2n+1\right)\sigma_{snh\to g}\sum_{k=0}^{n} R_n^k \psi_{nh}^k + \text{SOURCE TERMS} \quad .$$

Here

$$R_n^k = \sqrt{\frac{(2-\delta_{k0})\,(n-k)!}{(n+k)!}}\, P_n^k(\eta) \;\; \cos k\omega \quad ,$$

and

$$\int_{-1}^{1} d\eta \int_{0}^{\pi} d\omega R_n^k(\eta,\omega)\, R_m^\ell(\eta,\omega) = \frac{2\pi}{2n+1}\delta_{nm}\delta_{k\ell} \quad .$$

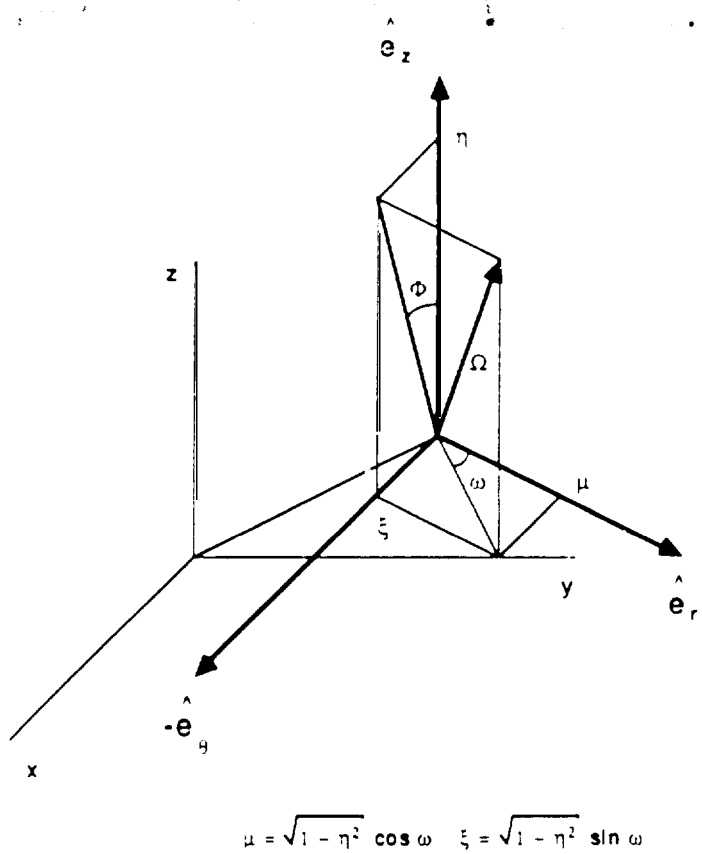

Fig. 1. Coordinates in (r,z) Geometry.

The expansion coefficients ψ_n^k are given by

$$\psi_n^k = \int_{-1}^{1} d\eta \int_{0}^{\pi} d\omega R_n^k \frac{\psi}{2\pi} \quad .$$

Now, if the transport equation is multiplied by R_m^ℓ and integrated over all angle, the analytic-balance equation for the R_m^ℓ moment is obtained. The orthogonality of the spherical harmonic functions R reduces the scattering sum on the right---hand side of the transport equation to

$$\sum_{h=1}^{G} \sigma_{smh\rightarrow g} \psi_{mh}^\ell \quad .$$

Now, the R_m^ℓ moment equation will be obtained using the discrete-ordinate-transport equation in place of the analytic form. In order to generate the R_m^ℓ moment-balance equation, the discrete-ordinate-transport equation is rnultiplied **by**

$$w_p R_m^\ell \left(\eta_p, \omega_p \right) \quad ,$$

and summed over all discrete directions p. If the discrete representation is to correctly model the analytic result, then the discrete directions must be chosen such that all the products

$$R_n^k R_m^\ell n, m \leq N \quad ; \quad k \leq n \quad ; \quad \ell \leq m \quad ,$$

arc integrated correctly! If this is the case, then the orthogonality of the R functions is preserved.

III. CHEBYSHEV-LEGENDRE QUADRATURE SET

The integral operator for integration over a11 solid angle is given by

$$\int_0^\pi sin\ \phi\ d\phi \int_0^{2\pi} d\omega \quad .$$

If $cos\ \phi = \eta$ and $cos\ \omega = y$, then the integral becomes

$$2 \int_{-1}^{1} d\eta \int_{-1}^{1} \frac{1}{\sqrt{1-y^2}} dy \quad .$$

It is well known that the y integration can be accomplished accurately with the equal weight Gauss-Chebyshev quadrature set. In fact, polynomials in y up to y^m, where $m \leq 2n_c - 1$, are integrated exactly (here n_c order of the Chebyshev quadrature). In a similar fashion, the η integral is exact for polynomials up to η' when the Gauss–Legendre quadrature set is used. $\ell \leq 2n_L - 1$ where n_L is the order of the Legendre quadrature set.

In the y integral, the quadrature points are given by

$$y_i = cos\ \omega_i,\ \omega_i = \frac{(2i-1)\,\pi}{2n_c} \quad , \quad i = 1, \cdots, n_c \quad .$$

The equal weights are

$$w_{ci} = \frac{\pi}{n_c} \quad .$$

The weights and quadrature points for the Legendre quadrature set are well known and are tabulated.

Notice that the values of ω are equally spaced between 0 and 2π. If the weights for the y integration are normalized by dividing by 2π, and the weights in the η integration arc normalized by dividing by 2, then the normalized Chebyshev weights w_c and the normalized Legendre weights w_L are given by

$$w_{ci} = \frac{1}{n_c} \quad , \quad w_{Lj} \rightarrow \frac{w_{Lj}}{2} \quad , \quad i = 1, \cdots, n_c \quad ; \quad j = 1, \cdots, n_L \quad .$$

The point weights associated with the two-dimensional integration is then the product of the j-th η level Legendre weight and the i-th Chebyshev weight. For a true product set that is consistent, we take $n_c = n_L = n_q$. n_q will be chosen an even integer. This is the square or product Chebyshev-Legendre quadrature set.

Will this quadrature set correctly integrate

$$\int_{-1}^{1} d\eta \int_{0}^{\pi} d\omega R_n^k(\eta,\omega)\, R_m^\ell(\eta,\omega) = \frac{2\pi}{2n+1}\delta_{nm}\delta_{k\ell} \quad ,$$

for all n, k, ℓ, and $m \le N$ where N is the scattering order? The answer is yes! Integrals of the form

$$\int_{0}^{\pi} cos\ k\omega\ cos\ \ell\omega d\omega \quad k+\ell \le 2N \quad ,$$

can be written

$$2\int_{-1}^{1} \frac{ay^1 + by^2 + \cdots + cy^{k+1}}{\sqrt{1-y^2}} dy \quad .$$

Notice that the integrand is now a polynomial in y of maximum order $k+1$. This can be shown by noting that

$$cos\ k\omega = a\,(cos\ \omega)^k + b\,(cos\ \omega)^{k-2} + \cdots + c\,(cos\ \omega)^M \quad ,$$

and since y = cos kw

$$cos\ kw = ay^k + by^{k-2} + \ldots + cy^M \quad .$$

Here, M = 0 for k even and M = 1 for k odd.

Since the integral over w leads to a $\delta_{k\ell}$, the integral over η has the form

$$\int_{-1}^{1} P_n^k(\eta)\, P_m^k(\eta)\, d\eta \quad , \quad n+m \le N \quad .$$

The highest power of η appearing in the integrand of the integral above is η^{n+m}, and the integrand is a polynomial in η.

Now, if the quadrature n_q is related to the scattering order by $n_q = N+1$, then the integration is exact for polynomial integrands of order $2n_q - 1$ or $2N+1$. The integrands involved are polynomials of maximum order 2N; hence, the integrals are computed exactly! This means, for example, that an S4 Chebyshev-Legendre (C-L) square or product quadrature will treat exactly P3 scattering.

IV. RESULTS AND CONCLUSIONS

The square geometry and the cross sections for each of the two sample problems is shown in Fig. 2. The leakage problem has a small absorption cross section while the average flux problem is a pure scattering problem. A plot of the differential scattering cross section for both problems is shown in Fig. 3. Notice that both differential cross sections arc strongly forward peaked.

Figure 4 is a plot of the average flux in the system as a function of the number of discrete-ordinate directions for the average flux cross--section set. Figure 5 is a plot of total leakage as a function of the number of discrete-ordinate directions for the leakage cross sections. In average flux problem, the current production set, which is the default set in TWODANT, yields divergent results for both S4 and S6 ordinates. Convergence finally occurs at S8 or forty directions. The square C-I, quadrature set yields a reasonable value with only 16 directions (S4 square set). The triangular C-L set is similar to the square C-I, set but uses Chebyshev integration of order 2 (2 points) on the η level with the largest value of η, Chebyshev integration of order 4(4 points) on the η level with the next largest value of η, and so on. In two dimensions, an SN square set has N^2 points and an SN triangle set has (N)(N + 2)/2 points. The triangular set can rigorously only yield correct results for Pl scattering. It can be seen from the results; however, that the triangular set, result approaches the square set result as the number of directions becomes large. The current production set, which is also a triangular set, seems to exhibit a constant offset with respect to the C-L sets even for a large number of directions (up to S16). Similar observations apply for the leakage results shown in Fig. 5.

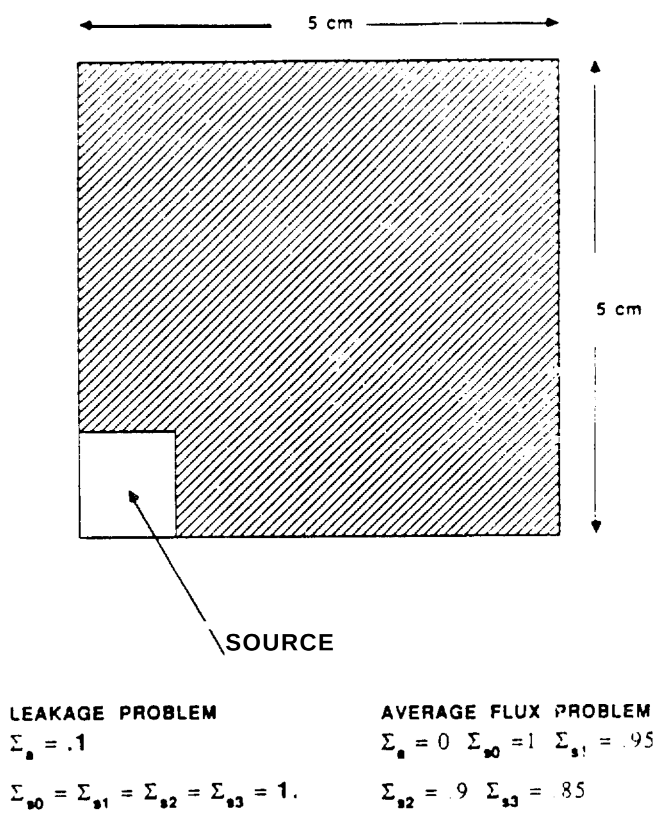

Fig. 2. Test Problem Geometry.

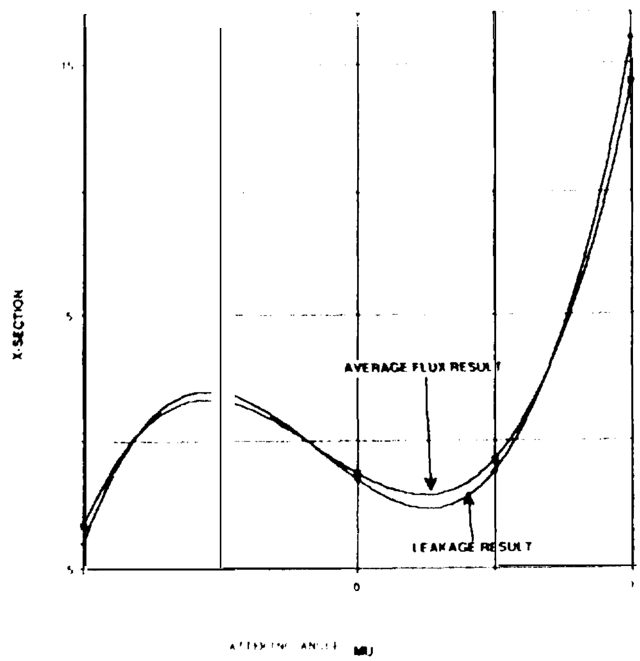

Fig. 3. Scattering X-Section vs. Angle Cosine.

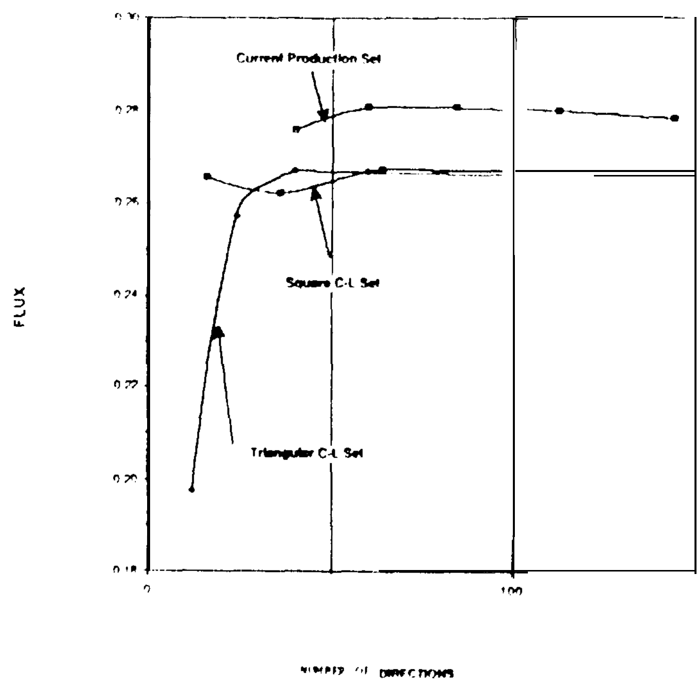

Fig. 4. Average Flux vs. Number of Directions.

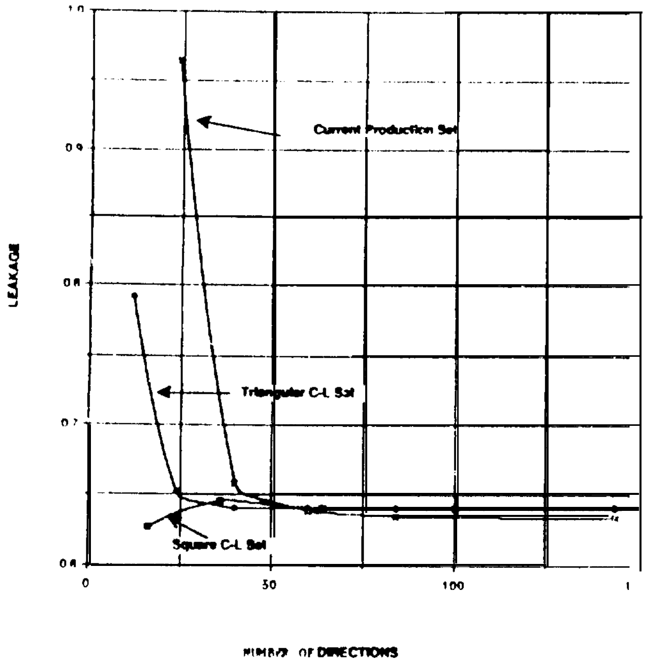

Fig. 5. Leakage vs. Ordinate Directions.

In Fig. 6 and the excess reactivity, multiplication constant **-1,** is plotted versus the number of discrete directions for a pure uranium cylinder. **P3** scattering is assumed. In Fig. **7,** the transport correction to the self-scatter cross section has been used to make the comparison easier. The transport correction has little or no effect on the C-L set, but results in a smoother result for the TWODANT production set. Again, the C-L set approaches the asymptotic result more quickly as the angular mesh is refined as compared to the production set. A constant offset is once again seen between the two sets.

The new square C-L quadrature set yields results in agreement with the default quadrature set in TWODANT when anisotropic scattering is small. The C-I, set is seen to be significantly better than the default set in problems where forward peaked scattering is large. If there is any question that high-order P3 scattering is important, the S4 square C-L set should be used instead of the S8 default set. The S4 square C-L set consists of 16 directions while the default S8 set consists of 40 directions. This difference will result in a large savings in storage and a decrease by a factor of 2.5 in the neutronic run time.

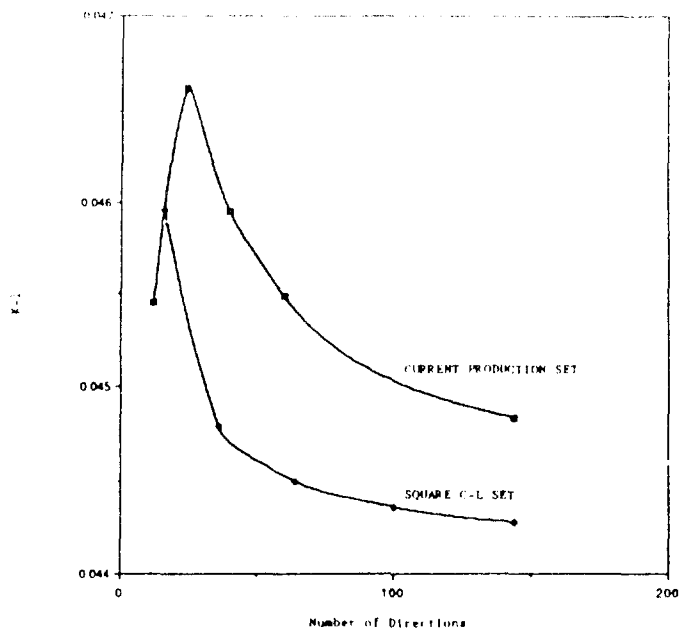

Fig. 6. Excess Reactivity vs. Discrete Directions.

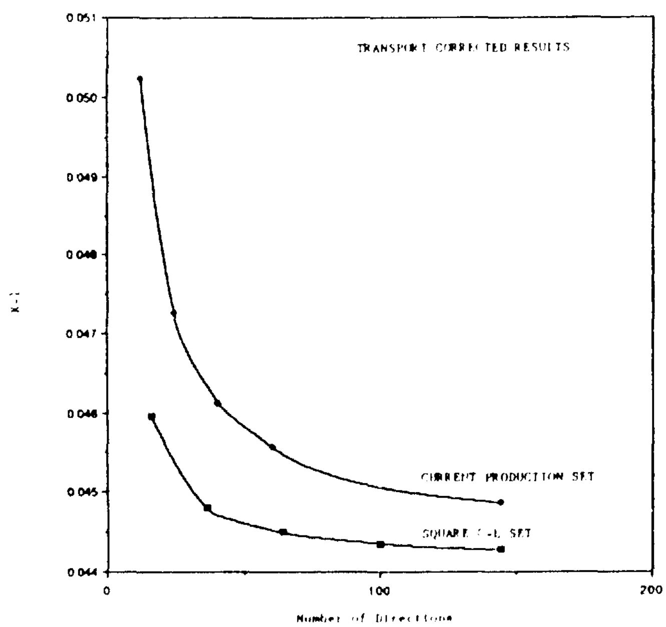

Fig. 7. Excess Reactivity vs. Discrete Directions-Transport Corrected Results.

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