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LOS ALAMOS SCIENTIFIC LABORATORY
OF THE UNIVERSITY OF CALIFORNIA ○ LOS ALAMOS NEW MEXICO

MECHANICAL QUADRATURE
AND THE TRANSPORT EQUATION

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MECHANICAL QUADRATURE AND THE TRANSPORT EQUATION

by

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Abstract

Methods of quadrature over the unit sphere with emphasis on rotational symmetry are discussed briefly in this report in relation to the problem of integrating the Neutron Transport Equation over the angular variable. Tables of quadrature coefficients are given for a particular method having the desired symmetry properties, and for two other methods.

In the solution of the neutron transport equation, the integration over the angular (directional) variable is usually performed by means of mechanical quadrature. The continuous angular variable Ω is, in other words, replaced by a set of discrete directions (Ω_s) to which is attached a set of weights (p_s). The directions may be represented as a set of points on the unit sphere.

When the above notions are imposed on the transport equation, a <u>set</u> of partial differential equation results, depending upon the variables time, neutron velocity, position in space, but <u>not</u> on the particle direction.

The first transport theory method, which was based on mechanical quadrature, was developed about 20 years ago. It is generally referred to as the Method of Discrete Ordinates or the Wick-Chandrasekhar Method. It has been applied mainly to the simple geometries (those with one space variable) where the azimuthal component of Ω often can be eliminated. In that event, the set (Ω_s) becomes a set of direction cosines (μ_m) and the point weights sum to a set of level weights (w_m). When this method is used with particular sets of discrete directions it often goes under other names such as the P_{n-1} Method or the Double $P_{n/2-1}$ Method $(DP_{n/2-1})$, to mention the two most familiar variants. Here n is the number of directions chosen. Both P_{n-1} and $DP_{n/2-1}$ are based on Gauss mechanical quadrature, i.e., on the zeroes (μ_m) of the Legendre polynomials of the first kind and the weights associated with these (w_m). Note that these zeroes are located symmetrically about $\mu=0$.

During the last few years the Angular Segmentation (or S_n) Method has been developed at this Laboratory. It is a general scheme for writing transport difference equations suitable for machine calculation and, as far as the angular variable is concerned, a generalization of the Method of Discrete Ordinates. S_n includes, therefore, as special cases, P_{n-1} and $DP_{n/2-1}$. In fact, for infinite plane geometry the S_n method differs from these other methods only in the procedure for determining μ_m and w_m. The DSN (or S_n) computer code can, therefore, in this case and others, be used for P_{n-1} or $DP_{n/2-1}$ calculations by simply changing quadrature coefficients.

The first S_n equations which were derived (1953) - for transport problems with one space dimension - did not result from the explicit assumption of a quantized angular variable. Later, the equations were found to imply a discrete respresentation of that variable, but one which was not symmetric about $\mu=0$. After a number of unsatisfactory results had been observed and the difficulty had been identified, another difference scheme was developed [1] satisfying the symmetry

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1) Carlson, Bengt; Numerical Solution of Transport Problems, Proceeding of Symposia in Applied Mathematics, vol. XI, pp. 219-232. See also LA-reports LA-2260 and LAMS-2346.

condition mentioned above and adequate, therefore, at least for problems with one space dimension.

To carry out integrations in one or more space dimensions, a directional mesh is superimposed on the orthogonal space mesh. Figuratively speaking, this is done as follows: The unit sphere - with points which define directions - is first supplied with three mutually perpendicular axes and then placed - lined up with the space mesh - at all mesh intersections. We now want the points on the unit sphere to be invariant with respect to all rotations by multiples of 90°. If they are not, the results of integrations will depend on the orientation of the sphere, which is clearly undesirable, and the neutron distributions are likely to be seriously distorted which is unacceptable. We have observed this in some cases. The distributions may, for instance, lack the simple symmetries which may be induced by geometrical ones.

We want then the points $\Omega_s = (\mu_i, \mu_j, \mu_k)$ to be symmetrically located with respect to the three poles (corners) of a unit sphere octant and to be duplicated on the other octants. Unfortunately this cannot be done using zeroes of orthogonal sets of polynomials. The symmetry requirement implies that the equation

$$(1) \qquad \mu_i^2 + \mu_j^2 + \mu_k^2 = 1$$

be satisfied with μ's selected from a set (μ_m), $m = 1, 2, \ldots, (n/2)$, and with $k = (n/2) + 2-i-j$, n even. By direct substitution in (1) one can verify that

(2) $$\mu_m^2 = \mu_1^2 + (m-1)\ \Delta$$

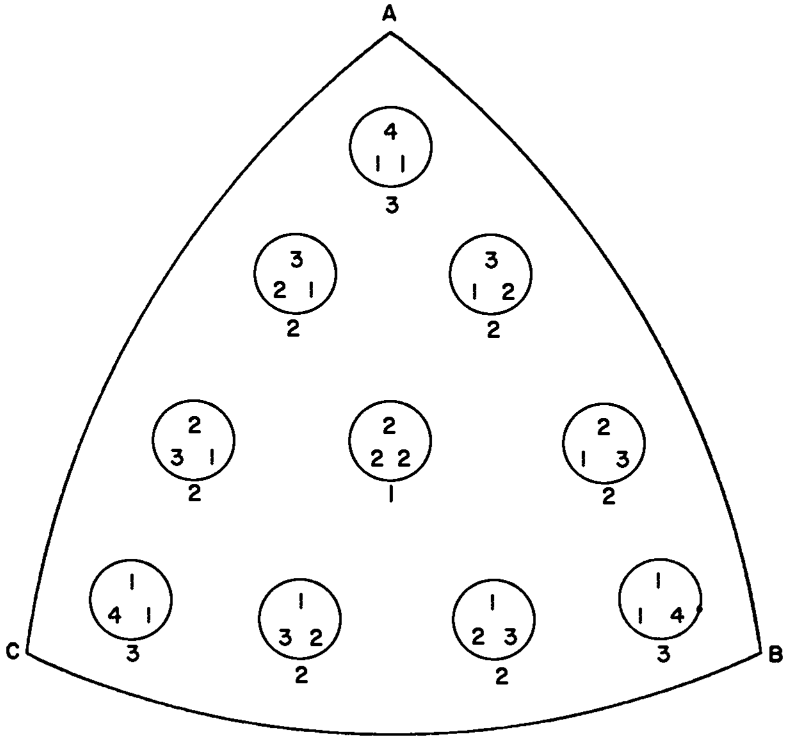
with μ_1^2 arbitrary and with

(3) $$\Delta = 2(1-3\mu_1^2)/(n-2)$$

satisfy (1) subject to the stated conditions. The degrees of freedom typical of quadratures based on orthogonal polynomials are, therefore, not present. Given μ_1^2, the other direction cosines are determined by (2) and (3).

For quadrature of order n we have n basic directions μ_m obtained from (2), using both signs, and a total of n(n+2) points on the sphere. This total is reduced if spacial symmetries are present, the minimum number (n) occurring in the one-dimensional plane and spherical geometries.

The figure drawn below (for n=8) illustrates the placement of the points on the octant and the conventions. The coordinates of the point $\binom{1}{14}$, for example, are measured with respect to the corners $\binom{A}{CB}$, and given by (μ_1, μ_1, μ_4). Note that the μ's are numbered starting at the side opposite the corner with respect to which they are measured. The point indices (s) are given underneath the circles.



Symmetry also requires that the weights p_s be equal when the coordinate triplets are equal. Hence, referring to the figure above, the weights p_3 for the corner points should be equal, likewise the weights p_2 of the six points about the center.

In general the points subdivide in groups of three types: A, B, and C. Type A points have unequal indices and come in groups of six. Type B points have two indices equal and come in groups of three. Finally, we may have one Type C point, a center point with equal indices, if n=8, 14, 20,....

The level weights w_m are defined as sums over the point weights, summed over points by rows with respect to any one of the corners. For n=8 we have $w_1=2p_2+2p_3$, $w_2=p_1+2p_2$, $w_3=2p_2$, and $w_4=p_1$.

Using the classification by types and relation (1), it can readily be shown, provided $\Sigma w_m = 1$, that

$$(4) \qquad \Sigma\, w_m\, \mu_m^{\;2} = 1/3,$$

and that

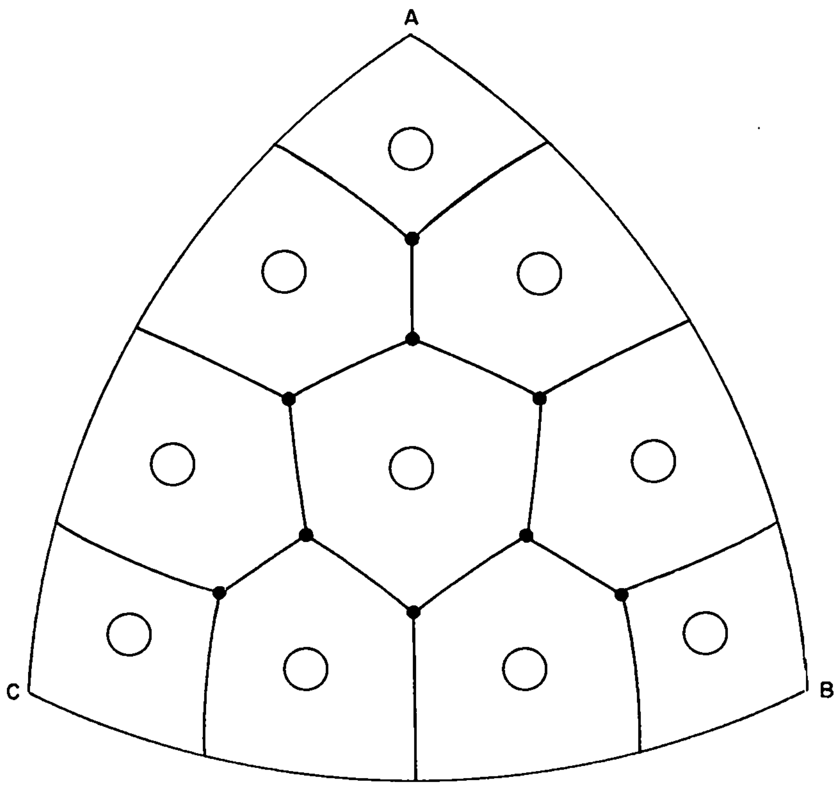
$$(5) \qquad \Sigma\, [(n/2) - m]\, w_m = \Sigma\, W_m = (n-2)/3,$$

where $W_{m+1} = W_m + w_m$, $m = 1, 2, \ldots, n/2-1$, with $W_1 = w_1$.

It is possible to determine $\mu_1^{\;2}$ and the $(n/2)-1$ independent weights w_m so that a set of moments are satisfied. We have not found a set of moments conditions, however, which result in w_m and p_s all positive for n up to at least 64. The work on this approach is continuing.

Here we describe an area method for determining p_s and hence w_m. We first choose $\mu_1^{\;2} = 1/3(n-1)$, based on an asymptotic theory. The latter, developed in analogy with the one for Legendre polynomials, says that $W_m \sim \bar{\mu}_m$, $m \neq n/2$, where $\bar{\mu}_m^{\;2} = \mu_1^{\;2} + (m - 1/2)\,\Delta$. This leads to an equation for $\mu_1^{\;2}$, using relation (5), which is satisfied by $\mu_1^{\;2} = 1/3(n-1)$ for n=2, and n=4, and also in the limit of large n. For intermediate n-values $\mu_1^{\;2} = 1/3(n-1)$ is very close but not precise.

Areas about the points on the spherical octant are then constructed as follows: Two direction cosines are inserted (by linear interpolation in μ^2) between all pairs of adjoining $\mu_m^{\;2}$. A set of auxiliary points on the unit sphere results, essentially a set of "midpoints" for all the "triangles" formed by the principal points. The auxiliary points are then connected with great circles segments and segments drawn to the octant boundaries are drawn in perpendicular fashion. The schematic diagram below (for n=8) illustrates the procedure. The principal points are indicated by small circles, the auxiliary ones by dots.



As can be deduced from this figure, one obtains "hexagons" in the central region, "houses" along the boundaries, and "squares" at the corners. The construction yields the required symmetry for the weights p_s. The algebra and arithmetic necessary for computing the separate areas are lengthy but otherwise simple. The S_n quadrature coefficients resulting from this method are given in the tables which follow. These contain also directions and weights for the P_{n-1} and $DP_{n/2-1}$ methods.* Schematic diagrams illustrating the point numbering conventions are given at the end of the report.

A more detailed account of the quadrature procedures introduced here and comparisons between these and other methods in simple transport problems will be given in a forthcoming LA report.[2)]

* The tables were prepared by Josephine Powers in Group T-1 of the Laboratory.

2. Lee, Clarence E., "The Discrete S_n Approximation to the Transport Equation", LA report (to be issued).

Table of Direction Cosines (μ_i) and Quadrature Weights (w_i) for Angular Segmentation (S_n), Spherical Harmonics (P_{n-1}), and Double Spherical Harmonics ($DP_{\frac{n}{2}-1}$).

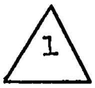
	m	w_m	μ_m	μ_m^2	n_s	p_s
S_2	1	1.00000000	.57735027	.33333333	1	1.00000000
P_1	1	1.00000000	.57735027	.33333333		
S_4	1	.66666667	.33333333	.11111111	3	.33333333
	2	.33333333	.88191710	.77777778		
P_3	1	.65214515	.33998104	.11558711		
	2	.34785485	.86113631	.74155574		
DP_1	1	.50000000	.21132487	.04465820		
	2	.50000000	.78867513	.62200846		
S_6	1	.49419458	.25819889	.06666667	3	.17247209
	2	.34494417	.68313005	.46666667	3	.16086125
	3	.16086125	.93094934	.86666667		
P_5	1	.46791394	.23861919	.05693912		
	2	.36076157	.66120939	.43719786		
	3	.17132449	.93246951	.86949939		
DP_2	1	.27777778	.11270167	.01270167		
	2	.44444444	.50000000	.25000000		
	3	.27777778	.88729833	.78729833		
S_8	1	.41554696	.21821789	.04761905	1	.07316139
	2	.27550683	.57735027	.33333333	6	.10117272
	3	.20234545	.78679579	.61904762	3	.10660076
	4	.10660076	.95118973	.90476190		
P_7	1	.36268378	.18343464	.03364827		
	2	.31370665	.52553241	.27618431		
	3	.22238103	.79666648	.63467748		
	4	.10122854	.96028986	.92215662		
DP_3	1	.17392742	.06943184	.00482078		
	2	.32607258	.33000948	.10890626		
	3	.32607258	.66999052	.44888730		
	4	.17392742	.93056816	.86595710		

Table Continued.

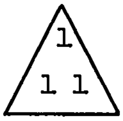
	m	w_m	μ_m	μ_m^2	n_s	p_s
S_{12}	1	.33208881	.17407766	.03030303	3	.03027563
	2	.21355025	.46056619	.21212121	3	.03473744
	3	.15130324	.62764591	.39393939	6	.04537599
	4	.12548941	.75878691	.57575758	6	.05689986
	5	.11379973	.87038828	.75757576	3	.06376856
	6	.06376856	.96922337	.93939394		
P_{11}	1	.24914704	.12533341	.01570846		
	2	.23349254	.36783150	.13530001		
	3	.20316743	.58731795	.34494237		
	4	.16007833	.76990267	.59275012		
	5	.10693932	.90411726	.81742802		
	6	.04717534	.98156063	.96346127		
DP_5	1	.08566224	.03376524	.00114009		
	2	.18038079	.16939531	.02869477		
	3	.23395697	.38069041	.14492519		
	4	.23395697	.61930959	.38354437		
	5	.18038079	.83060469	.68990415		
	6	.08566224	.96623476	.93360961		
S_{16}	1	.28532856	.14907120	.02222222	3	.01534259
	2	.18100812	.39440532	.15555556	3	.01763140
	3	.12803470	.53748385	.28888889	6	.01862861
	4	.10526928	.64978629	.42222222	3	.02328516
	5	.09192110	.74535599	.55555556	6	.02733194
	6	.08337745	.82999331	.68888889	6	.03004615
	7	.07954919	.90676470	.82222222	6	.03977459
	8	.04551160	.97752522	.95555556	3	.04551160
P_{15}	1	.18945061	.09501251	.00902738		
	2	.18260342	.28160355	.07930056		
	3	.16915652	.45801678	.20977937		
	4	.14959599	.61787624	.38177104		
	5	.12462897	.75540441	.57063582		
	6	.09515851	.86563120	.74931737		
	7	.06225352	.94457502	.89222196		
	8	.02715246	.98940093	.97891420		
DP_7	1	.05061427	.01985507	.00039422		
	2	.11119052	.10166676	.01033613		
	3	.15685332	.23723380	.05627988		
	4	.18134189	.40828268	.16669475		
	5	.18134189	.59171732	.35012938		
	6	.15685332	.76276620	.58181227		
	7	.11119052	.89833324	.80700261		
	8	.05061427	.98014493	.96068408		

Numbering of Directions when Plotted on Octant of Unit Sphere

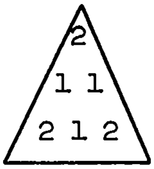
Schematic Diagrams



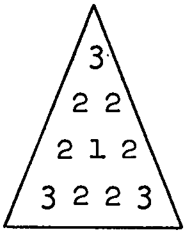
n=2



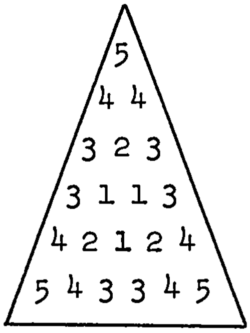
n=4



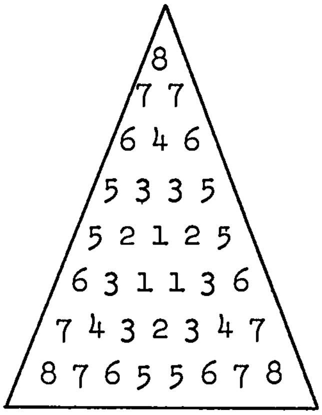
n=6



n=8



n=12



n=16