OPTIMUM ANGULAR SEGMENTATIONS IN NEUTRON TRANSPORT ANALYSIS

A.A. Harms and W.J. Garland
Department of Engineering Physics
McMaster University
Hamilton, Ontario, Canada

Abstract

The problem of specifying optimum angular segmentations in neutron transport analysis is considered. A new directional-group representation using partial-range Legendre polynomials is introduced for this purpose. It is found that this solution formalism can be used to specify angular segmentations which minimize the error of certain neutron transport parameters for a given order of approximation.

Introduction

The analytical study of one-speed neutron transport has been important in providing general descriptions of neutron migration(1,2). Increasingly, researchers are focussing attention on the development of computational strategies and on the extension of mathematical constructs to extend the utility of neutron transport models to a wider class of reactor physics problems.

One key problem which exists is the specification of angular segments in such neutron transport calculations. Though the initial application of the spherical harmonics method by Wick(3) and Mark(4) involved continuous expansions over the angular interval from -1 to +1, it was found by Yvon(5) that independent expansions over each of the half-ranges permitted substantial calculational improvements. More recently it has been shown(6) that partial-range Legendre polynomials can be defined over arbitrary partial ranges of the angular variable. This progression from full-range to half-range and now to partial-range representations has introduced an additional generalization; for example, both, Carlsons' S_N formalism(7) and the method using quadrature sets(8) can, in a sense, be considered as special cases of the partial-range representation(6).

Here, we examine specifically the problem of specifying "optimum" angular segmentations for neutron transport calculations. The criterion to be employed is the accuracy with which a transport parameter can be calculated for a given order of approximation. The analytical freedom in specifying angular segmentations of the partial-range Legendre polynomial representation, hereafter referred to by the acronym NP_L, is the motivation for using this formalism. To provide a sufficiently rigorous test, and also for reasons of historical precedent, we calculate the several tranport parameters associated with a vacuum-medium interface; the selected parameters are (1) the extrapolated end point, (2) the linear extrapolation length, (3) the asymptotic flux to total flux ratio and (4) the asymptotic decay constant.

In the following sections we first describe the partial-range formalism within the context of an arbitrary angular segmentation. Thereafter, we examine a low order approximation to illustrate certain characteristics of the formalism. Subsequently, we study in greater detail a higher order approximation. In the final section we summarize certain general rules for the specification of optimum angular segmentations.

Development of Model

Using the notation of Case and Zweifel[2], we write the one-speed integro-differential neutron transport equation for the case of isotropic scattering in source-free infinite plane geometry as

$$\mu\frac{\partial\psi}{\partial x}(x,\mu)+\psi(x,\mu) = \frac{c}{2}\int_{-1}^{1}\psi(x,\mu')d\mu' \ , \tag{1}$$

where μ represents the cosine of the scattering angle, x denotes the spatial variable in units of mean-free-path, and c denotes the number of secondary neutrons emitted per neutron-nucleus interaction. The angular neutron density is represented by $\psi(x,\mu)$.

Since the angular variable μ is defined over the range $(-1,+1)$, we impose N ordered angular segments over this domain as follows:

$$(-1,\mu_1),(\mu_1,\mu_2),\ldots,(\mu_{n-1},\mu_n),\ldots,(\mu_{N-1},+1) \ . \tag{2}$$

Over each of these segments we specify a linear partial-range variable, which, for the n'th interval, is defined by

$$\mu_n^* = \left(\frac{2}{\mu_n-\mu_{n-1}}\right)\mu - \frac{\mu_n+\mu_{n-1}}{\mu_n-\mu_{n-1}} \ . \tag{3}$$

We note here that μ_n^* is normalized in the sense that

$$\mu_n^* = -1 \text{ for } \mu = \mu_{n-1}, \text{ and } \mu_n^* = +1 \text{ for } \mu = \mu_n. \tag{4}$$

Next, we define partial-range Legendre polynomials over each angular segment by

$$P_{n,\ell}(\mu) = \begin{cases} P_\ell(\mu_n^*), & \mu_{n-1} < \mu < \mu_n \ , \\ 0, & \text{otherwise,} \end{cases} \tag{5}$$

and propose to write the solution to Eq. (1) in a form similar to the usual method associated with orthogonal polynomials:

$$\psi(x,\mu) = \sum_{n=1}^{N}\sum_{\ell=0}^{L}\frac{2\ell+1}{2}\phi_{n,\ell}(x)P_{n,\ell}(\mu) \ . \tag{6}$$

Further, we write the spatial moments $\phi_{n,\ell}(x)$ contained in this expression as

$$\phi_{n,\ell}(x) = A_{n,\ell}e^{-x/\nu} \tag{7}$$

Thus, the coefficients, $A_{n,\ell}$, and the eigenvalues, $1/\nu$, need to be found. Conditions for the $A_{n,\ell}$'s and the $1/\nu$'s are obtained by using the several properties of orthogonality, recurrence, and full-range integration(6). With the aid of these properties we substitute Eq. (6) and Eq. (7) into Eq. (1) to obtain a linear system of which the typical equation is given by

$$A_{n,\ell}\left(\frac{1}{\nu}\right)(\mu_n+\mu_{n-1})+A_{n,\ell-1}\left(\frac{\ell}{2\ell+1}\right)\left(\frac{1}{\nu}\right)(\mu_n-\mu_{n-1})-2A_{n,\ell}$$

$$+A_{n,\ell+1}\left(\frac{\ell+1}{2\ell+1}\right)\left(\frac{1}{\nu}\right)(\mu_n-\mu_{n-1})+c\sum_{n=1}^{N}A_{n,\ell}(\mu_n-\mu_{n-1})\delta_{0\ell} = 0 \quad . \tag{8}$$

with $n = 1,2,\ldots,N$ and $\ell = 0,1,2,\ldots,L$.

Lowest Order Approximation (N = 2)

In the preceeding section we have illustrated the derivation of a formalism which is particularly amenable to an emphasis on the angular segmentation. In this section we illustrate an application using this directional freedom to obtain an optimum segmentation in the sense of permitting a best possible estimate of the asymptotic decay constant. To make the analysis more obvious we choose the low order case of $N = 2$ and $L = 0$. This specifies two angular segments, namely $(-1,\mu_1)$ and $(\mu_1,+1)$. The problem, therefore, is the determination of μ_1 which yields the most accurate determination of the asymptotic decay constant for this order of approximation.

For the approximation desired, $N = 2$ and $L = 0$, the system of equations represented by Eq. (8) reduces to

$$A_{1,0}\{(1/\nu)(\mu_1-1)-2+c(\mu_1+1)\}+A_{2,0}\{c(1-\mu_1)\} = 0 \quad ,$$

$$A_{1,0}\{c(\mu_1+1)\}+A_{2,0}\{(1/\nu)(1+\mu_1)\}-2+c(1-\mu_1)\} = 0 \quad . \tag{9}$$

Since the coefficients $A_{1,0}$ and $A_{2,0}$ are of secondary interest at the present, we employ the usual methods of linear algebra to obtain here a 2x2 secular determinant in c, $1/\nu$ and μ_1. In this case, this determinant reduces to a quadratic equation in both $1/\nu$ and μ_1:

$$(\mu_1/\nu)^2-(1/\nu)+4(\mu_1/\nu)(c-1)-4(c-1) = 0 \tag{10}$$

We must now choose μ_1 subject to the following optimality criterion:

$$\mathrm{Min}|1/\nu-1/\nu_o| \text{ for all } c \quad . \tag{11}$$

Here, $1/\nu_o$ is the exact asymptotic decay constant(2) given by

$$1/\nu_o = \tanh^{-1}(1/\nu_o). \tag{12}$$

We have performed this analysis by numerical search. In Table 1 we show the results for this $2P_0$ approximation and, in addition, we have extended this analysis to the next approximation with $N = 2$ and $L = 1$, i.e. $2P_1$. For purpose of ready comparison, we list in the same table the results obtainable from the usual methods of spherical Harmonics for $L = 3$, i.e. P_3. This comparison illustrates that, while the difference between the NP_L and P_L results are small for higher c, a substantial improvement is possible with decreasing c. Indeed, even in the low order approximations examined here, an angular segmentation can be specified which approaches the exact value of the asymptotic decay constant for the case of heavily absorbing media.

Higher Order Segmentation

The principal complexity brought about in the calculation of neutron transport parameters using an optimum angular segmentation in a higher order approximation is attributed to the appearance of eigenvalues in the secular determinant associated with Eq. (8). This requires that the spatial moments be expanded in all these eigenvalues as follows

$$\phi_{n,\ell}(x) = \sum_{j=1}^{N} \sum_{k=0}^{L} B_{j,k} A_{n,\ell}(\nu_{j,k}) e^{-x/\nu_{j,k}} \quad . \tag{13}$$

Here, we have indicated the dependence of $A_{n,\ell}$ on $\nu_{j,k}$; the $B_{j,k}$'s are constants to be found by the use of boundary conditions appropriate to the problem considered.

As the class of angular segmentations to be considered in detail we specify the following three partitions

$$(-1,0),(0,\mu^{o}),(\mu^{o},+1), \text{ and } (-1,\mu^{o}),(\mu^{o},0),(0,+1) \quad , \tag{14}$$

where μ^{o} is the optimum angular segmentation to be identified. This specifies $N = 3$. We further choose to restrict ourself here to $L = 1$; this therefore defines the $3P_1$ approximation.

For this case of $N = 3$ and $L = 1$, the formal solution of Eq. (1), which incorporates Eq. (13) and Eq. (6), is now written

$$\psi(x,\mu) = \sum_{n=1}^{3} \sum_{\ell=0}^{1} \frac{2\ell+1}{2} P_{n,\ell}(\mu) \left[\sum_{j=1}^{3} \sum_{k=0}^{1} B_{j,k} A_{n,\ell}(\nu_{j,k}) e^{-x/\nu_{j,k}} \right] \quad . \tag{15}$$

The several neutron transport parameters to be evaluated require the evaluation of the neutron scalar flux

$$\psi(x) = \int_{-1}^{1} \psi(x,\mu')d\mu' \quad , \tag{16}$$

and the asymptotic flux[9]

$$\psi_{asy}(x) = \sum_{n=1}^{3} \frac{\mu_n - \mu_{n-1}}{2} \left[B_- A_{n,0}(\nu_-) e^{-x/\nu_-} + B_+ A_{n,0}(\nu_+) e^{-x/\nu_+} \right] \quad . \tag{17}$$

Both expressions follow directly from the definitions of $\psi(x,\mu)$. In this latter expression we define $1/\nu_-$ as the largest negative eigenvalue and $1/\nu_+$ as the smallest positive eigenvalue; we further introduce the normalization that $B_- = 1$.

The three neutron transport parameters which we will evaluate computationally are typically associated with a vacuum-medium interface and defined by the following:

1) Extrapolated end point Z_0;

$$\psi_{asy}(Z_o) = 0 \; . \tag{18}$$

2) Linear extrapolation length λ;

$$\lambda = \frac{\psi_{asy}(0)}{\psi'_{asy}(x)\rceil_{x=0}} \; . \tag{19}$$

3) Ratio of the asymptotic flux to the total flux,

$$\Phi = \frac{\psi_{asy}(0)}{\psi(0)} \; . \tag{20}$$

In Table II we list typical results from this calculation. In the upper part, for c = 0.5, we show that by a suitable choice of the angular segmentation μ^o it is possible to obtain exact values for these neutron transport parameters even in this low order approximation. We note, however, that the angular segmentation differs somewhat for the several parameters. In the lower part, for c = 0.7, we show the best estimates of the neutron transport parameters which can be obtained by an optimum choice of the angular segmentation μ^o. Again, by direct numerical comparison, it has been found that these results are as accurate or more accurate than can be obtained with the Double-P_L and P_L formalism for comparable orders of approximation.

Discussion and Conclusion

In the preceding section we described the analytical formalism of the NP_L representation and illustrated the computational improvements possible with an optimum angular segmentation. From Table I we can extract, for example, the general rule of specifying an optimum angular segmentation which, for a given c, will permit the most accurate determination of the asymptotic decay constant in the $2P_0$ and $2P_1$ approximation. As is clear, the angular segmentation should be close to $\mu_1 = \pm 1.0$ as c decreases; the rate of change depends upon the approximation used.

We have further undertaken to specify rules for the determination of an optimum angular segmentation, μ^o, in the $3P_1$ approximation applicable to the other neutron transport parameters. As is evident from the results listed in Table II, the rules differ non-linearly and depended upon both, the number of secondary neutrons, c, and the specific parameter, Φ, Z_o and λ. An overall pattern may, however, be graphically represented, Fig. 1. Here we show the domain from which μ^o should be extracted as a function of c which lead to, either the exact value, or the best estimate, of the neutron transport parameters Φ, Z_o and λ.

Acknowledgment

Financial support in this work by the National Research Council of

Canada is gratefully acknowledged.

References

1. B. Davison, "Neutron Transport Theory", Oxford University Press, London, (1957).

2. K.M. Case and P.F. Zweifel, "Linear Transport Theory", Addison-Wesley Publ. Co., Reading, Mass., (1967).

3. G.C. Wick, Physics, 121, 702, (1943).

4. J.C. Mark, MT-92, National Research Council of Canada, (1944).

5. J. Yvon, J. Nucl. Energy, 1, 4, 304, (1957).

6. A.A. Harms, Can. J. Physics, 48, 1007, (1970).

7. B.G. Carlson, LA-1891, Los Alamos Scientific Laboratory, (1955).

8. K.O. Lathrop and B.G. Carlson, LA-3186, Los Alamos Scientific Laboratory, (1965).

9. M.M.R. Williams, "Mathematical Methods in Particle Transport Theory", Wiley-Interscience, New York, (1971).

c	$1/\nu_o$ (Exact)	$1/\nu$ for $2P_o$ (this work)	$1/\nu$ for $2P_1$ (this work)	$1/\nu$ for P_3 (Spherical Harmonics)
.1	1.0000	1.0000 ($\mu_1 = \pm.99$)	1.0000 ($\mu_1 = \pm.99$)	1.139
.2	.9999	1.0000 ($\mu_1 = \pm.99$)	1.0000 ($\mu_1 = \pm.99$)	1.113
.4	.9856	1.0000 ($\mu_1 = \pm.99$)	.995 ($\mu_1 = \pm.90$)	1.040
.6	.9073	.980 ($\mu_1 = \pm.82$)	.917 ($\mu_1 = \pm.66$)	.923
.8	.7104	.800 ($\mu_1 = \pm.50$)	.714 ($\mu_1 = \pm.42$)	.712
.9	.5254	.600 ($\mu_1 = \pm.34$)	.527 ($\mu_1 = \pm.28$)	.526

Table I: Tabulation of asymptotic decay constant and associated angular segmentation for $2P_o$ and $2P_1$ as derived herein and comparison to results obtainable using P_L (Spherical Harmonics) with L = 3.

c = 0.5			
Parameter	Exact Value	Calculated (this work: $3P_1$)	Error %
Φ	1.176	1.176 (μ^o = .905)	0
Z_o	1.441	1.441 (μ^o = .921)	0
λ	.920	.920 (μ^o = .999)	0

c = 0.7			
Parameter	Exact Value	Calculated (this work: $3P_1$)	Error %
Φ	1.206	1.202 (μ^o = .79)	.33
Z_o	1.018	1.005 (μ^o = .79)	1.29
λ	.830	.812 (μ^o = .79)	2.17

Table II: Neutron transport parameters and their associated optimum angular segmentation for the $3P_1$ approximations.

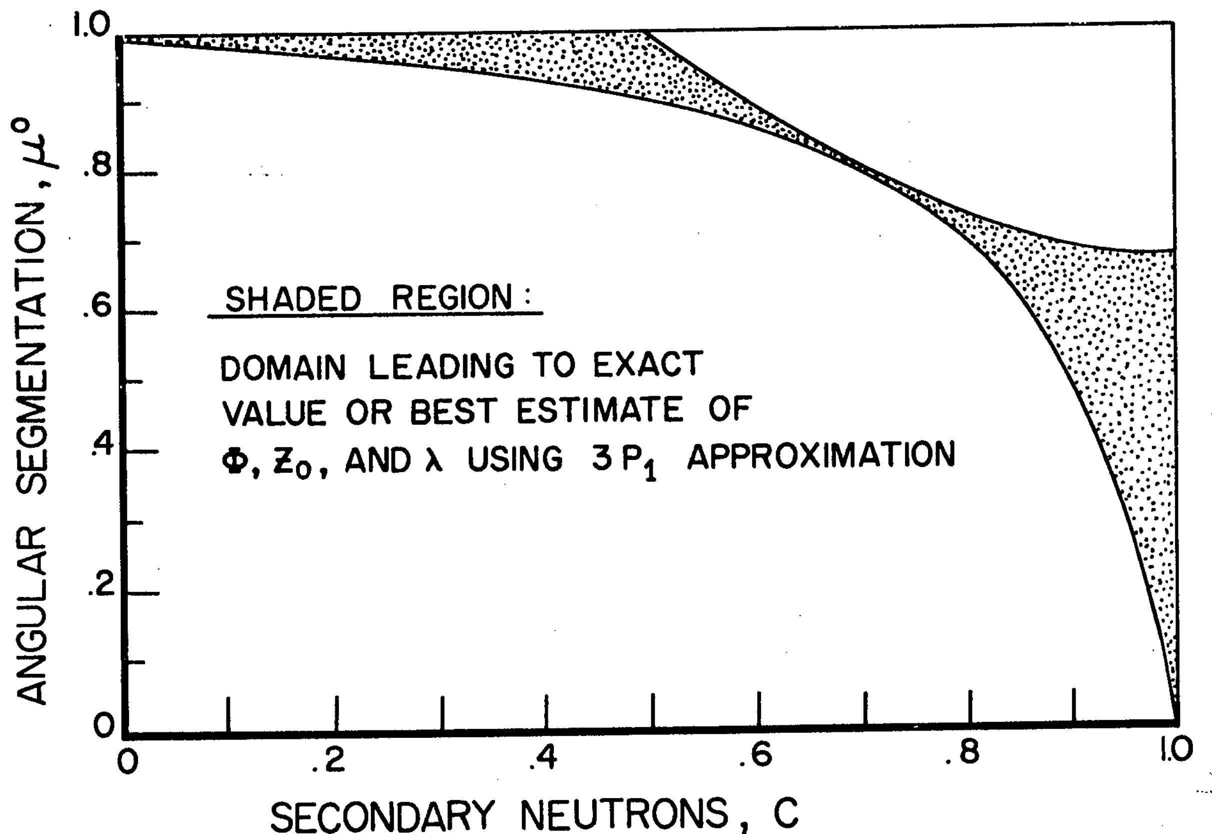

Fig. 1: Results of $3P_1$ analysis which specifies the domain of the angular segmentation μ^o as a function of the number of secondary neutrons which lead either to the exact or best estimate of (1) the asymptotic to total flux ratio Φ, (2) the extrapolated end point Z_o and (3) the linear extrapolation length λ.