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A Review of Neutron Transport Approximations

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Numerical methods for solving the integrodifferential, integral, and surface-integral forms of the neutron transport equation are reviewed. The solution methods are shown to evolve from only a few basic numerical approximations, such as expansion techniques or the use of quadrature formulas. The emphasis is on the derivation of the approximate equations from the transport equation, and not on the solution of the resulting system of algebraic equations.

The presentation covers the approaches used in general-purpose production calculations, including the discrete ordinates finite difference method, the method of characteristics, finite element approximations, the collision-probability method, and nodal methods. Various quasi-analytical techniques for calculating benchmark problems are also treated, such as the singular eigenfunction, spherical harmonics, integral transform, and C_N and F_N methods.

I. OVERVIEW

I.A. Introduction

The particle transport equation used in radiation shielding and reactor core calculations, as well as radiative transfer analysis of stellar and planetary atmospheres, is a linearized version of the equation originally developed by Boltzmann for the kinetic theory of gases. The fundamentals of such transport phenomena are available in several monographs.[1-7]

Except for highly idealized problems, solution of the transport equation is accomplished by numerical means. A large variety of numerical methods have been developed which, at first glance, appear quite different. Upon further inspection, however, it may be seen that these methods are based on a few approximation techniques, such as finite differences for differential operators, quadrature formulas for integral operators, or expansion methods.

It is the purpose of this paper to present in detail the basic principles of the approximations used to solve the neutron transport equation. One of our motivations is to tie together the various solution methods within the framework of numerical approximation techniques; the emphasis is on the derivation of the approximate equations from the transport equation, and not on the solution of the resulting system of algebraic equations. The presentation is limited to deterministic methods for the one-group, steady-state transport equation, with the exclusion of the stochastic Monte Carlo technique. Energy dependence is not treated in an explicit way, but the techniques discussed here apply, for the most part, to the multigroup formalism; for completeness, a brief discussion of iterative schemes used in the solution of the multigroup equations is given in the Appendix.

[1]K. M. CASE, F. de HOFFMANN, and G. PLACZEK, *Introduction to the Theory of Neutron Diffusion*, U.S. Government Printing Office, Washington, D.C. (1953).

[2]S. CHANDRASEKHAR, *Radiative Transfer*, Oxford University Press, London (1950) and Dover, New York (1960).

[3]B. DAVISON, *Neutron Transport Theory*, Oxford University Press, London (1957).

[4]K. M. CASE and P. F. ZWEIFEL, *Linear Transport Theory*, Addison-Wesley Publishing Co., Inc., Reading, Massachussetts (1967).

[5]C. CERCIGNANI, *Mathematical Methods in Kinetic Theory*, Plenum Publishing Company, New York (1969).

[6]M. M. R. WILLIAMS, *Mathematical Methods in Particle Transport Theory*, Butterworths, London (1971).

[7]J. J. DUDERSTADT and W. R. MARTIN, *Transport Theory*, John Wiley & Sons, Inc., New York (1979).

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The choice of the numerical method differs according to whether the solution involves a highly idealized "benchmark" problem or a more realistic "production" problem such as the calculation of the neutron flux in an optically large region of a reactor or a shield. For a given problem, the choice of the method depends on the degree of information required for the spatial and angular dependence of the neutron distribution. The choice also depends on the approximations one uses to describe the properties of the media and their geometrical configuration; for example, this includes the degree of anisotropy of the scattering, the complexity of the material heterogeneities, and the optical size of each homogeneous region. (Perhaps, most importantly, the choice depends on which computer programs are readily available!)

Solutions of the neutron transport equation are obtained using one of three formulations: the integrodifferential, the integral, and the surface-integral forms. The choice among the three is determined by physical and numerical considerations. Generally the integrodifferential approach is used for the treatment of optically large media, whereas the methods based on the integral equation are most appropriate in calculations for optically thin media. When only the angular fluxes leaving and entering a media are desired, the surface-integral approach may be advantageous. The general criteria concerning numerical solutions are the computer-memory requirements, the computer time needed to calculate the matrix elements, the computer time used to solve the system of algebraic equations, and the rate of convergence of the method.

The integrodifferential equation is based on a local neutron balance, and leads to sparse matrices whose elements are easily computed. Usually these matrices are solved by an iterative procedure that requires that only a small part of the matrix be stored in central memory at a given time. On the other hand, the integral equation is derived from a global neutron balance in a given direction and therefore it is strongly coupled. This coupling leads to full matrices whose elements must be calculated by numerical integration involving expensive evaluation of transcendental functions; the algebraic system of equations must be solved globally and a complete matrix must be kept in central memory. The surface-integral method is based on the Placzek lemma,[1] which relates the transport solution for a finite geometry problem to that for an infinite medium; a numerical approximation of this equation in one-dimensional geometries yields a system of algebraic equations for the angular fluxes at the surfaces.

The integrodifferential and integral equation methods can be compared for the degree of geometrical detail that can be attained. General-purpose production methods based on the integrodifferential form of the transport equation utilize either a geometrical mesh or finite elements, and therefore any configuration can be approximated, even though a large number of zones are sometimes required to achieve good geometrical modeling. On the other hand, integral equation methods are inherently limited because they require a different specialized subroutine for numerical integration in each configuration; however, they do provide an exact geometrical representation.

The integral equation methods offer an exact treatment of the angular dependence, provided the scattering anisotropy is low (isotropic or linearly anisotropic), whereas the integrodifferential equation methods require discretization of the angular variable. This discretization results in a strong coupling between the spatial and the angular approximations that can produce space-angular nuisances such as the ray effect. Also, it should be emphasized that integrodifferential methods require calculation of angular fluxes, whereas integral equation methods directly produce scalar fluxes (which usually is all that is needed). Consequently, smaller matrices are encountered for integral equation methods, which explains why a relatively small effort has been spent on the implementation of iterative solutions and development of acceleration techniques for these methods (see the Appendix).

With the integrodifferential and the surface-integral approaches, it is possible to treat an arbitrary degree of anisotropy of scattering by modifying the collision term, without unduly complicating the numerical solution. On the other hand, in the integral formulation the number of equations to be solved dramatically increases with the degree of anisotropy.

Nowadays the trend in the development of general-purpose transport methods is to combine the use of both the integrodifferential and integral equations. In these methods, the spatial domain is divided into subregions (usually homogeneous) that are linked together by the angular flux at the interfaces, as calculated with the integral equation. In the method of characteristics, for example, the integrodifferential equation is used to calculate the angular flux within the region in terms of the incoming angular fluxes, whereas in nodal methods the interior flux is usually computed with the integral equation. The advantages of such "hybrid" methods are twofold. First, since the integral equation is used to calculate the angular fluxes exiting from a subregion, neutron streaming is well approximated and this allows for larger size subregions than in a typical integrodifferential method calculation. Second, in contrast with the full coupling of integral equation methods, the interconnecting of subregions through only their interface angular fluxes leads to sparse matrices that are amenable to iterative solution.

In Secs. I.B. and I.C, we introduce our notation,

discuss the three forms of the transport equation, and present some of the ideas behind the numerical approximation techniques. The notation used in the description of most of the methods is not that in the original literature, but we believe this notation helps to bring out the similarities between the different methods that otherwise may be difficult to perceive. The reader already familiar with the fundamentals of transport theory and numerical approximations can skip over the next two sections and use them only as a reference for the basic equations and notation.

Section II covers the numerical methods based on the integrodifferential equation. We begin with three procedures, the singular eigenfunction method and the spherical-harmonics and analytic discrete ordinates approximations, used to obtain accurate solutions to benchmark problems in one-dimensional geometries. The latter two procedures are shown to be approximations to the formally exact singular eigenfunction method. The remainder of Sec. II is devoted to the methods used in general-purpose computer codes. First we discuss discrete ordinates methods: the well-known finite difference discrete ordinates approach and the relatively new method of characteristics. Then finite element methods are presented for both the ordinary and the even-parity form of the transport equation.

Integral equation methods are discussed in Sec. III. After a comparative evaluation of the discrete integral transport, collocation, and collision probability methods, we focus on the latter, which is the method most widely used in production codes. We consider the case of isotropic scattering and sources and describe the usual flat-flux approximation for the three one-dimensional and the two-dimensional Cartesian geometries; then the more general multifunction expansions are considered. The extension to linearly anisotropic scattering in one-dimensional geometries is then presented. We also briefly study the integral transform and the spatial spherical harmonics methods; these two methods are closely related to the collision probability formalism and have been used to obtain benchmark solutions to idealized problems in simple geometries. Finally, two nodal approaches are described in the last portion of Sec. III: the interface current method and the more recent transverse nodal method. Within the context of the interface current technique, response and transmission matrix methods are also briefly considered; all three techniques are currently used in general-purpose production codes. The transverse nodal approach also offers promise for use in production calculations.

Section IV contains a discussion of the complementarity (C_N) and facile (F_N) methods, both of which are based on the surface-integral form of the transport equation. These methods are used for benchmark calculations in one-dimensional geometries. General comments on all the methods based on the three forms of the transport equation are given in Sec. V.

In view of the extensive research on methods of solution of the transport equation, it would be nearly impossible to include a complete list of references; fortunately, comprehensive lists of references are in several conference proceedings[8-15] and books,[16-19] which cover the material discussed here. We particularly note the review articles by Froehlich[20] and by Lewis[21] and a recent book by Duderstadt and Martin[7] that is very thorough.

I.B. Three Forms of the Transport Equation

The expected steady-state monoenergetic distribution of neutrons propagating through matter or

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[8]*Proc. Conf. New Developments in Reactor Mathematics and Applications,* Idaho Falls, Idaho, March 29-31, 1971, CONF-710302, U.S. Atomic Energy Commission (1971).

[9]*Proc. Sem. Numerical Reactor Calculations,* Vienna, January 17-21, 1972, International Atomic Energy Agency (1972).

[10]*Proc. Conf. Mathematical Models and Computational Techniques for Analysis of Nuclear Systems,* Ann Arbor, Michigan, April 9-11, 1973, CONF-730414, U.S. Atomic Energy Commission (1973).

[11]*Proc. Conf. Computational Methods in Nuclear Engineering,* Charleston, South Carolina, April 15-17, 1975, CONF-750413, U.S. Energy Research and Development Administration (1975).

[12]*Proc. IAEA Specialists Mtg. Methods of Neutron Transport Theory in Reactor Calculations,* Bologna, Italy, November 3-5, 1975, CONF-751152, International Atomic Energy Agency (1976).

[13]*Proc. National Topl. Mtg. ANS Mathematics and Computation Division,* Tucson, Arizona, March 28-30, 1977, published in *Nucl. Sci. Eng.*, **64**, 1-709 (1977).

[14]*Proc. Topl. Mtg. Computational Methods in Nuclear Engineering,* Williamsburg, Virginia, April 23-25, 1979, CONF-790402, American Nuclear Society (1979).

[15]*Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems,* Munich, Germany, April 27-29, 1981, Kernforschungszentrum Karlsruhe (1981).

[16]M. CLARK and K. F. HANSEN, *Numerical Methods of Reactor Analysis,* Academic Press, Inc., New York (1964).

[17]H. GREENSPAN, C. N. KELBER, and D. OKRENT, Eds., *Computing Methods in Reactor Physics,* Gordon and Breach, Science Publishers, Inc., New York (1968).

[18]G. I. BELL and S. GLASSTONE, *Nuclear Reactor Theory,* Van Nostrand Reinhold Ltd., New York (1970).

[19]J. BUSSAC and P. REUSS, *Traité de Neutronique,* Hermann, Paris (1978).

[20]R. FROEHLICH, "Current Problems in Multidimensional Reactor Calculations," *Proc. Conf. Mathematics Models and Computational Techniques for Analysis of Nuclear Systems,* Ann Arbor, Michigan, April 9-11, 1973, CONF-730414, Vol. II, p. VII-1, Atomic Energy Commission (1973).

[21]E. E. LEWIS, *Nucl. Sci. Eng.* **64**, 279 (1977).

vacuum is described by the angular flux $\psi(\boldsymbol{r},\boldsymbol{\Omega})$, which gives the neutron density at a point $\boldsymbol{r}$ in direction $\boldsymbol{\Omega}$. We use the notation $x = (\boldsymbol{r},\boldsymbol{\Omega})$ to denote a point in phase space. The angular flux depends on the properties of the medium (characterized by cross sections) and the distribution and intensities of any external sources $S(x)$. If one is interested in only the distribution of neutrons within a given region of space D, the sources exterior to the region are usually replaced by boundary conditions that specify the incoming angular flux $\psi_-(x)$.

In the following, we denote by X the five-dimensional phase space $X = \{x = (\boldsymbol{r},\boldsymbol{\Omega}); \boldsymbol{r} \in D, \boldsymbol{\Omega} \in \mathcal{S}_2\}$ where $\mathcal{S}_2$ is the set of directions on the 4π unit sphere. That is, X contains all phase points $x = (\boldsymbol{r},\boldsymbol{\Omega})$ where $\boldsymbol{r}$ is a point within domain D and $\boldsymbol{\Omega}$ is the unit vector in the neutron direction. Likewise, designating by $\boldsymbol{n}(\boldsymbol{r})$ the outward normal at a point $\boldsymbol{r}$ on the boundary ∂D, we denote by $\partial X_\pm = \{x; \boldsymbol{r} \in \partial D, \pm\boldsymbol{\Omega}\cdot\boldsymbol{n} \geqslant 0\}$ the set of trajectories leaving (+) or entering (−) the domain D. In general, we use the symbols + and − to denote quantities associated with outgoing and incoming directions; for example, $x_\pm = (\boldsymbol{r},\boldsymbol{\Omega})$ represents a point on the boundary with an outgoing/incoming direction.

For conciseness, all integrals are understood to be over the entire domain of the variable unless otherwise indicated. Also, the arguments of the functions are stated the first time they appear, and omitted thereafter unless confusion could arise.

I.B.1. Integrodifferential Form

The stationary, monoenergetic transport of neutrons in a domain D with boundary ∂D is given by

$$B\psi = S \ , \quad \text{in } X \ ,$$
$$\psi = \psi_- \ , \quad \text{on } \partial X_- \ . \tag{1}$$

The transport operator

$$B = L - H \tag{2}$$

is composed of the spatial differential operator

$$L = \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} + \Sigma(\boldsymbol{r}) \ ,$$

which accounts for neutron streaming in direction $\boldsymbol{\Omega}$, and of the angular integral operator

$$H\psi = \int \Sigma_s(\boldsymbol{r},\boldsymbol{\Omega}' \to \boldsymbol{\Omega})\psi(\boldsymbol{r},\boldsymbol{\Omega}')d\boldsymbol{\Omega}' \ ,$$

which gives the distribution of neutrons appearing after a collision. The total macroscopic cross section Σ and the transfer cross section Σ_s characterize the interactions of neutrons with the medium.

Here we consider only media whose properties are invariant under rotation. For these isotropic media the transfer cross section depends on $\boldsymbol{\Omega}'$ and $\boldsymbol{\Omega}$ only through their product $\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}$; therefore, Σ_s can be expanded on the set of Legendre polynomials $P_k(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})$,

$$\Sigma_s(\boldsymbol{r},\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}) = (4\pi)^{-1}\sum_{k\geqslant 0}\Sigma_{sk}(\boldsymbol{r})P_k(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}) \ . \tag{3}$$

In practice, one uses for Σ_s a finite expansion extending from 0 to K, where K is the degree of anisotropy of the scattering kernel. It is customary to factorize the scattering coefficients as

$$\Sigma_{sk} = (2k+1)\Sigma c f_k \ ,$$

where Σ and $c(\boldsymbol{r})$ correspond to the probability of interaction per unit distance and to the mean number of secondaries following an interaction, respectively. The coefficient $f_k(\boldsymbol{r})$ is the k'th Legendre component of the scattering frequency $\Sigma_s/c\Sigma$; in particular, $f_0 = 1$ and f_1 is the mean cosine $\bar{\mu}$ of the scattering angle.

Because Σ_s is rotationally invariant, the collision operator H is also invariant under rotations and may be decomposed as

$$H = \sum_{k\geqslant 0}(2k+1)^{-1}\Sigma_{sk}Q_k \ . \tag{4}$$

Here Q_k is the orthogonal projection operator on the invariant subspace $\mathcal{E}_k$, which is spanned by the set of spherical harmonics $\{Y_k^l; |l| \leqslant k\}$,

$$Q_k\psi = \sum_{|l|\leqslant k} Y_k^l(\boldsymbol{\Omega})\int [Y_k^l(\boldsymbol{\Omega}')]^*\psi(\boldsymbol{r},\boldsymbol{\Omega}')d\boldsymbol{\Omega}' \ . \tag{5}$$

This operator satisfies the orthogonality and completeness properties

$$Q_kQ_l = \delta_{kl}Q_k \ ,$$

and

$$\sum_{k\geqslant 0} Q_k = 1 \ . \tag{6}$$

A particular case of later interest to us is that of plane geometry with azimuthally independent sources and boundary conditions; here the angular flux depends only on the spatial variable z and the cosine of the polar angle μ, so the collision operator H can be written as

$$H\psi = \Sigma(c/2)\sum_{k\geqslant 0}(2k+1)f_kP_k(\mu) \times \int P_k(\mu')\psi(z,\mu')d\mu' \ .$$

Then, with z measured in units of mean-free-paths, the transport equation takes the well-known form

$$(\mu\partial_z + 1)\psi(z,\mu) = \Sigma^{-1}H\psi + S(z,\mu) \ . \tag{7}$$

Now we consider the interface and boundary conditions. Since the cross sections are bounded, the angular flux within the medium must be continuous

at any point at which there are no localized sources. For a surface source on a surface Γ, integration of transport Eq. (1) yields the jump condition

$$\langle \psi(\cdot,\boldsymbol{\Omega}) \rangle = S_s(\boldsymbol{r},\boldsymbol{\Omega})/\boldsymbol{\Omega}\cdot\boldsymbol{n} \ , \quad \boldsymbol{r}\in\Gamma \ , \tag{8}$$

where the brackets denote the value of the discontinuity of the angular flux $\psi(\boldsymbol{r},\boldsymbol{\Omega})$ in the direction $\boldsymbol{n}$, and S_s is the magnitude of the surface source.

The angular flux ψ_- entering the boundary ∂D can be decomposed as

$$\psi_- = \psi_0 + \psi_h \ , \tag{9}$$

where ψ_0 is the inhomogeneous component and ψ_h is the homogeneous part, which we assume has the form[22]

$$\psi_h(x_-) = \beta\psi = \int \beta(x'_+ \to x_-)\psi(x'_+)dx'_+ \ . \tag{10}$$

Here $x_- = (\boldsymbol{r},\boldsymbol{\Omega}) \in \partial X_-$ and $x'_+ = (\boldsymbol{r}',\boldsymbol{\Omega}') \in \partial X_+$ are points in phase space with spatial coordinates $\boldsymbol{r}$ and $\boldsymbol{r}'$ on the boundary ∂D, and $\boldsymbol{\Omega}$ is an incoming direction while $\boldsymbol{\Omega}'$ is an outgoing one. The four-dimensional area element dx'_+ is the differential surface element $dA'd\boldsymbol{\Omega}'$ involving the element of surface area dA' on ∂D. Depending on the kernel $\beta(x'_+ \to x_-)$, a variety of boundary conditions can be represented, including reflection, translation, and periodic conditions. In practical calculations, the local reflection conditions often take the form

$$\beta(x'_+ \to x_-) = \begin{cases} \beta(\boldsymbol{r})\pi^{-1}(\boldsymbol{\Omega}'\cdot\boldsymbol{n})\delta_A(\boldsymbol{r}'-\boldsymbol{r}) \ , & \text{isotropic} \ , \\ \beta(\boldsymbol{r})\delta_2(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}_R)\delta_A(\boldsymbol{r}'-\boldsymbol{r}) \ , & \text{specular} \ , \end{cases} \tag{11}$$

where

$\beta(\boldsymbol{r})$ = local albedo

δ_A = delta function that reduces a volume integral to an integral over the two-dimensional surface ∂D

$\delta_2(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}) = (2\pi)^{-1}\delta(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega} - 1)$, i.e., the Placzek delta function[1]

$\boldsymbol{\Omega}_R = \boldsymbol{\Omega} - 2(\boldsymbol{\Omega}\cdot\boldsymbol{n})\boldsymbol{n}$.

A boundary condition that is often used in reactor cell calculations is that of uniform isotropic reflection (i.e., the "white" boundary condition), for which

$$\beta(x'_+ \to x_-) = \beta(\pi A)^{-1}(\boldsymbol{\Omega}'\cdot\boldsymbol{n}) \ . \tag{12}$$

[22]R. SANCHEZ, "Schemas Approchés de Résolution de l'Equation Intégrale du Transport à Deux Dimensions. Etude Théorique des Méthodes Mixtes de Résolution," CEA-N-2166, Commissariat à l'Energie Atomique (1980).

Here the albedo β is the fraction of neutrons reentering the body uniformly and isotropically, and A is the area of the surface ∂D. In this case, the reflected flux given by Eq. (10) can be written (in the usual notation) as

$$\psi_h(\boldsymbol{r},\boldsymbol{\Omega}) = \beta(\pi A)^{-1}\int dA \int_{2\pi+} (\boldsymbol{\Omega}'\cdot\boldsymbol{n})\psi(\boldsymbol{r},\boldsymbol{\Omega}')d\boldsymbol{\Omega}' \ ,$$

where the integral over $d\boldsymbol{\Omega}'$ is taken only for the outgoing directions $(\boldsymbol{\Omega}'\cdot\boldsymbol{n}) > 0$.

I.B.2. Integral Form

The integral equation is derived by integrating along the characteristics of the differential operator[1] (i.e., the neutron streaming trajectories) and can be written as

$$\psi = T(q + S_-) \ , \tag{13}$$

where the integral operator T,

$$Tf = \int t(x' \to x)f(x')dx'$$

$$= \int_D \int_{4\pi} t(\boldsymbol{r}',\boldsymbol{\Omega}' \to \boldsymbol{r},\boldsymbol{\Omega})f(\boldsymbol{r}',\boldsymbol{\Omega}')d\boldsymbol{r}'d\boldsymbol{\Omega}' \ ,$$

is the inverse of the differential operator L. The kernel t is the uncollided neutron angular flux at $x = (\boldsymbol{r},\boldsymbol{\Omega})$ due to a localized source at $x' = (\boldsymbol{r}',\boldsymbol{\Omega}')$, i.e., the uncollided angular flux at $(\boldsymbol{r},\boldsymbol{\Omega})$ produced by a unit source at $\boldsymbol{r}'$ in direction $\boldsymbol{\Omega}'$. Formally, this kernel is the Green's function solution of

$$\begin{aligned} Lt &= \delta(x' - x) \ , \quad \text{in } X \ , \\ t &= 0 \ , \quad \text{on } \partial X_- \ , \end{aligned} \tag{14}$$

where $\delta(x' - x) = \delta(\boldsymbol{r}' - \boldsymbol{r})\delta_2(\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})$. In Eq. (13),

$$q = H\psi + S = \int \Sigma_s(\boldsymbol{r},\boldsymbol{\Omega}' \to \boldsymbol{\Omega})\psi(\boldsymbol{r},\boldsymbol{\Omega}')d\boldsymbol{\Omega}' + S(\boldsymbol{r},\boldsymbol{\Omega}) \tag{15}$$

is the volumetric angular emission density, and the surface source S_- accounts for the boundary contributions,

$$S_- = -(\boldsymbol{\Omega}\cdot\boldsymbol{n})\psi_-\delta_-(x) \ . \tag{16}$$

Here we introduce the special delta functions

$$\int f(x)\delta_\pm(x)dx = \int f(x_\pm)dx_\pm \ .$$

When the domain D is convex, the uncollided angular flux also may be written as[4]

$$t(x' \to x) = \delta_2(\boldsymbol{\Omega}_s\cdot\boldsymbol{\Omega}')\frac{e^{-\tau}}{s^2}\delta_2(\boldsymbol{\Omega}_s\cdot\boldsymbol{\Omega}) \ . \tag{17}$$

In this expression, $\boldsymbol{s} = \boldsymbol{r} - \boldsymbol{r}'$, $\boldsymbol{\Omega}_s$ is the unit vector $\boldsymbol{s}/s$, and $\tau(\boldsymbol{r}',\boldsymbol{r})$ is the optical distance from $\boldsymbol{r}'$ to $\boldsymbol{r}$:

$$\tau = \int_0^s \Sigma(\boldsymbol{r}' + t\boldsymbol{\Omega}_s)dt \ .$$

Physically, the first factor in Eq. (17) indicates that only particles emitted in direction $\boldsymbol{\Omega}_s$ are followed, the second factor gives the geometric and material attenuation of the angular flux between $\boldsymbol{r}'$ and $\boldsymbol{r}$, and the third factor selects the appropriate direction $\boldsymbol{\Omega}$. With the aid of Eq. (17), the integral equation yields the well-known form

$$\psi = \int_0^{s_b} q(\boldsymbol{r} - s\boldsymbol{\Omega},\boldsymbol{\Omega})e^{-\tau}ds + \psi_-(\boldsymbol{r}_b,\boldsymbol{\Omega})e^{-\tau_-} \ , \quad (18)$$

where $\tau = \tau(\boldsymbol{r} - s\boldsymbol{\Omega},\boldsymbol{r})$, $\boldsymbol{r}_b$ is the point on the surface ∂D defined by $\boldsymbol{r}_b = \boldsymbol{r} - s_b\boldsymbol{\Omega}$, with $s_b \geqslant 0$, and $\tau_- = \tau(\boldsymbol{r}_b,\boldsymbol{r})$ is the optical distance from $\boldsymbol{r}_b$ to $\boldsymbol{r}$.

An equivalent way of constructing the integral form of the transport equation is to include the homogeneous component of boundary condition (9) in the Green's function. The new form of the integral equation is

$$\psi = \overline{T}(q + S_i) \ , \quad (19)$$

where the kernel of the integral operator $\overline{T}$ satisfies

$$L\bar{t} = \delta(x - x') \ , \quad \text{in } X \ ,$$
$$\bar{t} = \beta\bar{t} \ , \quad \text{on } \partial X_- \ .$$

The surface source S_i is given by Eq. (16) except that the surface contribution ψ_- in that equation is replaced by only the inhomogeneous part ψ_0.

In the case of white boundary condition (12), one can obtain a useful relation between Green's functions $\bar{t}$ and t, namely[22]

$$\bar{t}(x' \to x) = t(x' \to x) + (\pi A)^{-1} \exp[-\tau_+(x')]$$
$$\times [\beta/(1 - \beta P_{SS})] \exp[-\tau_-(x)] \ . \quad (20)$$

Here $\tau_\pm(x)$ denotes the optical distance in direction $\pm\boldsymbol{\Omega}$ from point $\boldsymbol{r}$ to the surface ∂D, and P_{SS} is the probability that neutrons, entering the body uniformly and isotropically, will escape without undergoing a collision:

$$P_{SS} = (\pi A)^{-1} \int (\boldsymbol{\Omega}\cdot\boldsymbol{n}) \exp[-\tau_-(x_+)]dx_+ \ . \quad (21)$$

In Eq. (20), the factor $(\pi A)^{-1} \exp[-\tau_-(x)]$ represents the uncollided angular flux at x produced by one neutron entering uniformly and isotropically the body, and the factor $\exp[-\tau_+(x')]$ is the uncollided escape probability from a source $\delta(x - x')$.

I.B.3. Surface-Integral Form

The steady-state neutron distribution within a body is uniquely defined by the incoming angular flux and by the internal sources.[4] This fact is used to derive the third form of the transport equation by relating (via Placzek's lemma) the flux within a homogeneous body to that in an infinite body.

Let us now assume a body D with boundary ∂D to be homogeneous and surrounded by vacuum and let ψ be the angular flux produced by all internal and external sources. Now suppose that the same homogeneous material fills all space, that the sources outside ∂D are suppressed, and that the artificial surface source

$$S_b = -(\boldsymbol{\Omega}\cdot\boldsymbol{n})\psi \int_{\partial D} \delta(\boldsymbol{r}' - \boldsymbol{r})dA'$$

is added. (The integral on the right side amounts to a delta function, which will reduce a volume integral into an integral over surface ∂D.) For $\boldsymbol{\Omega}\cdot\boldsymbol{n} < 0$, the source S_b reproduces the incoming angular flux of the original problem, while for $\boldsymbol{\Omega}\cdot\boldsymbol{n} > 0$ it equals the negative of the outgoing flux. When added to the outgoing angular flux, the net effect of the negative part of the surface source is to cancel out all neutrons leaving the system.

Since there are effectively no neutrons outside the original domain D, the angular flux solution (the one that vanishes at infinity) of the postulated infinite medium problem equals, within D, the solution ψ of the original problem. This allows us to express the desired solution ψ in terms of the infinite-medium Green's function

$$\psi = T_B(S + S_b) = \int_X t_B(x' \to x)$$
$$\times [S(x') + S_b(x')]dx' \ , \quad \text{in } X \ . \quad (22)$$

The integral operator T_B is the inverse of the transport operator B of Eq. (2); the kernel of T_B is the infinite medium Green's function satisfying the equation

$$Bt_B = \delta(x - x') \ , \quad \text{all } x$$
$$t_B \text{ bounded at } \infty \ .$$

This Green's function $t_B(x' \to x)$ is the total angular flux at $x = (\boldsymbol{r},\boldsymbol{\Omega})$ produced by a neutron emitted at $x' = (\boldsymbol{r}',\boldsymbol{\Omega}')$.

The final form of the surface-integral transport equation follows by specializing Eq. (22) to the points on the surface ∂D:

$$\psi = \int_X t_B(x' \to x)S(x')dx'$$
$$- \int_{\partial X} t_B(x' \to x)(\boldsymbol{\Omega}'\cdot\boldsymbol{n}')\psi(x')dx' \ , \quad \text{on } \partial X \ . \quad (23)$$

The second term in this equation, which is an integral on the boundary ∂D and in all directions, arises from the artificial surface source S_b. Once t_B is known, such a transport equation allows calculation of the angular flux on the surface of a medium without knowledge of the flux inside. For one-dimensional geometries, this infinite-medium Green's function can be computed in a straightforward manner.

I.C. Numerical Approximation Techniques

Any numerical approximation of the transport equation is the result of some discretization procedure such that

1. the angular flux function is replaced by a finite set of N values
2. the transport equation is replaced by a set of approximate algebraic equations for calculation of these values.

The technique used to derive this approximation may be based on a direct discretization of the transport operator, or on an expansion of the angular flux in terms of a finite set of functions, or on a combination of the two.

One of the desirable properties of a good numerical technique is that the approximate angular flux will "converge," with increasing values of N, to the true flux. Although convergence assures that the approximate solution for the angular flux ultimately will be everywhere positive and that local neutron balance will be preserved, it is highly desirable that these two properties hold even for small N.

By local neutron balance we mean the usual conservation equation satisfied by the total flux ϕ and the net current $\boldsymbol{J}$. This equation is obtained by direct integration of the transport equation over all directions,

$$\nabla \cdot \boldsymbol{J} = S_t - \Sigma_a \phi \ , \tag{24}$$

where S_t is the angle-integrated (total) source and Σ_a is the absorption cross section.

I.C.1. Expansion Methods

The three forms of the transport equation may be written formally as

$$M\psi = S \ , \quad \text{in } X \ ,$$

where M represents an operator acting on some space E of regular functions defined on domain X, and S is the source term. A numerical solution of this equation is equivalent to solving an approximate equation of the type[23,24]

$$\widetilde{M}\widetilde{\psi} = \widetilde{S} \ , \quad \text{in } X \ ,$$

in some finite N-dimensional space E_N, which is usually a subspace of E. This approximate solution $\widetilde{\psi}$ may be written as

$$\widetilde{\psi} = \sum_{n=1}^{N} \psi_n f_n \ , \tag{25}$$

where the $\{f_n, n = 1 \text{ to } N\}$ is a set of linearly independent functions spanning E_N. The determination of the expansion coefficients ψ_n is done in such a way as to minimize the residual ϵ obtained by substituting the approximate solution in the exact equation

$$\epsilon = M\widetilde{\psi} - S \ .$$

The nature of the expansion method depends on how this minimization is done. The collocation method consists of choosing N points $\{x_n \in X, n = 1 \text{ to } N\}$ and requiring that the residual identically vanish at these points. This results in the following set of algebraic equations for the evaluation of the expansion coefficients ψ_n:

$$\sum_{m=1}^{N} M_{nm}\psi_m = S_n \ , \quad n = 1 \text{ to } N \ , \tag{26}$$

where

$$M_{nm} = (Mf_m)(x_n) \ ,$$

and

$$S_n = S(x_n) \ .$$

This system of equations will give a solution if the collocation points x_n are selected so that the matrix of elements M_{nm} is not singular.

The projection technique, another scheme for constructing approximate equations, relies on the existence of a scalar product in space E of the form

$$(f,g) = \int fg dx \ , \quad f,g \in E \ .$$

In this technique, an N-dimensional subspace $F_n \subset E$ is selected, and the approximate equations are obtained by forcing to zero the projection of the residual onto F_N. If P denotes the orthogonal projection operator $P{:}E \to F_N$, then the approximate equations are given by

$$PM\widetilde{\psi} = PS \ . \tag{27}$$

In practice, the operator P can be constructed using a set $\{\xi_n, n = 1 \text{ to } N\}$ of orthonormal basis functions in F_N. For an arbitrary function f, the action of the projection operator P on f is given by

$$Pf = \sum_{n=1}^{N} (\xi_n, f)\xi_n \ .$$

With the aid of this expression, and the fact that the ξ_n are linearly independent, substitution of expansion (25) into Eq. (27) yields a set of equations of the form of Eq. (26) for the expansion coefficients ψ_n.

The approximation obtained with the projection

[23] L. V. KANTOROVICH and G. P. AKILOV, *Functional Analysis in Normed Spaces,* Pergamon Publishing Corporation, Oxford (1964).

[24] M. A. KRASNOSEL'SKII, G. M. VAINIKKO, P. P. ZABREIKO, Ya.B. RUTITSKII, and V.Ya. STETSENKO, *Approximate Solutions of Operator Equations,* Wolters-Noordhoff, Groningen (1972).

technique is generally called the weighted residual approximation. The particular case of interest here, called the Galerkin-Petrov method,[24] results from the choice $F_N = E_N$, for which

$$M_{nm} = (f_n, Mf_m)$$

and

$$S_n = (f_n, S)$$

in Eq. (26). Hereafter, this approximation is simply referred to as the projection method.

I.C.2. Quadrature Method

To complete this discussion, we need to consider the numerical methods obtained from the use of a quadrature formula of the form

$$\int f(\mathbf{r})d\mathbf{r} \sim \sum_{n=1}^{N} V_n f(\mathbf{r}_n) \ , \qquad (28)$$

where the $\{\mathbf{r}_n, V_n, n = 1 \text{ to } N\}$ are, respectively, the nodes and positive weights of the integration formula. Use of this formula for a constant function shows that the sum of the V_n yields the total volume V, so the weights V_n may be interpreted as the volumes associated with the nodes.

Such a quadrature formula can be used, for example, to obtain a numerical approximation for an integral equation

$$\phi = G\phi + S \ , \qquad (29)$$

with integral operator G. After use of the quadrature formula to evaluate $G\phi$, and after specialization of the resulting equation to the nodes $\mathbf{r}_n$, one obtains[25]

$$\phi_n = \sum_{m=1}^{N} g(\mathbf{r}_m \to \mathbf{r}_n) V_m \phi_m + S_n \ , \quad n = 1 \text{ to } N \ , \qquad (30)$$

where $g(\mathbf{r}' \to \mathbf{r})$ is the kernel of the operator G and $S_n = S(\mathbf{r}_n)$. This system of equations gives the approximate values $\phi_n = \phi(\mathbf{r}_n)$ of the unknown function ϕ at the nodes of integration. Equation (30) also can be viewed as the result of using the "expansion"

$$\phi(\mathbf{r}) = \sum_{n=1}^{N} \phi_n V_n \delta(\mathbf{r} - \mathbf{r}_n)$$

in the collocation method with collocation points $\{\mathbf{r}_n\}$.

Whenever the kernel $g(\mathbf{r}' \to \mathbf{r})$ is singular the $g(\mathbf{r}_n \to \mathbf{r}_n)$ are not defined. However, when this kernel is integrable, one way of circumventing this difficulty is to rewrite Eq. (29) in the form

$$(1 - G1)\phi = \int g(\mathbf{r}' \to \mathbf{r})[\phi(\mathbf{r}') - \phi(\mathbf{r})]d\mathbf{r}' + S \ , \qquad (31)$$

provided that the integral

$$(G1)(\mathbf{r}) = \int g(\mathbf{r}' \to \mathbf{r})d\mathbf{r}'$$

can be obtained analytically. Then the previous procedure yields

$$[1 - (G1)(\mathbf{r}_n)]\phi_n = \sum_{\substack{m=1 \\ m \neq n}}^{N} g(\mathbf{r}_m \to \mathbf{r}_n) V_m(\phi_m - \phi_n) + S_n \ ,$$

$$n = 1 \text{ to } N \ .$$

II. INTEGRODIFFERENTIAL EQUATION METHODS

In this section, we consider five well-known methods for solving the integrodifferential transport equation. In the first, the singular eigenfunction method, the angular flux is calculated in terms of solutions of the homogeneous transport equation. For plane geometry, these solutions are obtained by separating the spatial and angular variables with the substitution $\phi_\nu(\mu) \exp(-z/\nu)$; this results in a homogeneous Fredholm integral equation of the second kind for $\phi_\nu(\mu)$. The novelty of the method is that a complete set of eigenfunctions can be obtained by including solutions that correspond to the continuous spectrum of the operator.

The common feature of the spherical harmonics and the discrete ordinates methods is that an approximation is used to eliminate the integral term of the transport operator. This results in a set of differential equations that are handled by classical numerical techniques[26,27] or, in plane geometry, by analytical methods. In the spherical harmonics method, the integral term is treated by expanding the flux in terms of eigenfunctions of the integral operator, i.e., the spherical harmonics. After truncation of the expansion, this approximation yields a set of coupled ordinary differential equations for the expansion coefficients.

In the discrete ordinates approximation, a numerical quadrature in the angular variable is used to simplify the integral term of the transport equation. This results in a set of coupled ordinary differential

[25]L. M. DELVES and J. WALSH, Eds., *Numerical Solutions of Integral Equations,* Clarendon Press, Oxford (1974).

[26]H. G. KAPER and G. K. LEAF, "A Survey of Approximation Procedures for the Numerical Solution of the Neutron Transport Equation," ANL-7779, Argonne National Laboratory (1971).

[27]K. D. LATHROP, "Transport Theory Numerical Methods," *Proc. Conf. Mathematics Models and Computational Techniques for Analysis of Nuclear Systems,* Ann Arbor, Michigan, April 9-11, 1973, CONF-730414, Vol. I, p. I-1, Atomic Energy Commission (1973).

equations for the angular fluxes in the directions specified by the quadrature formula; these equations are solved by a finite difference technique (the most widely used integrodifferential method) or by the method of characteristics. In both cases, the domain is decomposed into homogeneous cells within a geometrical mesh and a conservation equation is used to relate the fluxes within a cell. In the finite difference approach, the conservation relation is supplemented with auxiliary relations (such as the diamond difference approximation). In the method of characteristics, on the other hand, an integration along neutron trajectories is used to relate outgoing and incoming angular fluxes for a cell.

The finite element method has been adapted, in the last decade, from other fields of engineering to treat the angular and/or spatial variable in neutron transport problems. This method can be viewed as a projection technique in which the flux is expanded locally on piecewise polynomials.

II.A. Singular Eigenfunction Expansions

The singular eigenfunction expansion method is a formally exact technique for solving the integrodifferential transport equation. The primary usefulness of the method is in the understanding of the mathematical structure of the equation and the general behavior of its solutions. The method is closely related to the Wiener-Hopf,[3,28] resolvent integration,[29,30] and transmission matrix methods.[31-33]

Our interest here in the singular eigenfunction method is only to show how the method is related to other numerical methods, although in fact this formally exact method has been used for benchmark calculations that require the numerical evaluation of Cauchy principal-value integrals.

The method is modeled after the Fourier approach to partial differential equations: the solution of the transport equation in each homogeneous region of the medium is written as the sum of a particular solution and a linear combination of solutions of the homogeneous transport operator.[4,34] The homogeneous part of the solution is selected so that the interface and external boundary conditions are satisfied. A key step in the procedure is the construction of a complete set of solutions of the homogeneous transport equation. In fact, this problem is so difficult that only in simple one-dimensional geometries has the technique been used for numerical calculations.

The essence of the method can be understood by considering the case of plane geometry given by Eq. (7). In this geometry, the spatial and angular variables may be separated with the *ansatz* $\phi_\nu(\mu)\exp(-z/\nu)$. The result is

$$(\nu - \mu)\phi_\nu = (c\nu/2)g(\nu,\mu) \ , \tag{32}$$

where

$$g(\nu,\mu) = (2/c)\Sigma^{-1}H\phi_\nu = \sum_{k\geq 0}(2k+1)f_k g_k(\nu)P_k(\mu) \ . \tag{33}$$

The $g_k(\nu)$ is the k'th Legendre component of ϕ_ν, i.e.,

$$g_k(\nu) = \int_{-1}^{1} P_k(\mu)\phi_\nu(\mu)d\mu \ . \tag{34}$$

The formal solution of Eq. (32) may be written as

$$\phi_\nu = \frac{c}{2}\frac{\nu}{\nu - \mu}g(\nu,\mu) + \lambda(\nu)\delta(\nu - \mu) \tag{35}$$

where, when performing integrals over ν or μ, the integral of the first term is to be interpreted as a Cauchy principal value integral.[35,36] Since Eq. (32) is homogeneous in ϕ_ν, we can select the normalization condition

$$\int_{-1}^{1}\phi_\nu(\mu)d\mu = g_0(\nu) = 1 \ . \tag{36}$$

The remaining $g_k(\nu)$ are calculated by multiplying Eq. (32) by $P_k(\mu)$ and integrating over $-1 \leq \mu \leq 1$. This gives the recursion relation

$$(k+1)g_{k+1}(\nu) - \nu h_k g_k(\nu) + k g_{k-1}(\nu) = 0 \tag{37}$$

with the coefficients

$$h_k = (2k+1)(1 - cf_k) \ .$$

As a consequence of the normalization condition and the recursion relation, the $g_k(\nu)$ are polynomials of order k, alternatively even and odd; in particular, this implies that $g(-\nu,-\mu) = g(\nu,\mu)$. For a purely absorbing medium ($c = 0$), the $g_k(\nu)$ reduce to the Legendre polynomials. A compact expression for the $g_k(\nu)$ is

[28]M. M. R. WILLIAMS, *Advances in Nuclear Science and Technology*, Vol. 7, p. 283, E. J. HENLEY and J. LEWINS, Eds., Academic Press Inc., New York (1973).

[29]E. W. LARSEN and G. J. HABETLER, *Comm. Pure Appl. Math.*, **26**, 525 (1973).

[30]W. GREENBERG and P. F. ZWEIFEL, *Transp. Th. Stat. Phys.*, **5**, 219 (1976).

[31]R. ARONSON, *Nucl. Sci. Eng.*, **27**, 271 (1967).

[32]R. ARONSON, *Transp. Theory Stat. Phys.*, **1**, 209 (1971).

[33]G. CAROLL and R. ARONSON, *Nucl. Sci. Eng.*, **51**, 166 (1973).

[34]N. J. McCORMICK and I. KUŠČER, *Advances in Nuclear Science and Technology*, Vol. 7, p. 181, E. J. HENLEY and J. LEWINS, Eds., Academic Press Inc., New York (1973).

[35]F. D. GAKHOV, *Boundary Value Problems*, Pergamon Press, Oxford (1966).

[36]B. W. ROOS, *Analytic Functions and Distributions in Physics and Engineering*, John Wiley & Sons Inc., New York (1969).

given by the determinant[37]

$$g_{k+1}(\nu) = \frac{1}{(k+1)!} \begin{vmatrix} h_0\nu & 1 & 0 & 0 & . & . & 0 \\ 1 & h_1\nu & 2 & 0 & . & . & 0 \\ 0 & 2 & h_2\nu & 3 & . & . & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & . & k & h_k\nu \end{vmatrix} , \quad k \geq 0 . \quad (38)$$

The values ν for which Eq. (35) is a valid solution of the transport equation are fixed by the normalization condition. From Eqs. (35) and (36), we obtain a continuous spectrum $[-1,1]$ and a set of discrete eigenvalues. These eigenvalues are the roots of the function

$$\Lambda(\nu) = 1 - \frac{c}{2}\nu \int_{-1}^{1} \frac{g(\nu,\mu)d\mu}{\nu - \mu} . \quad (39)$$

This function is analytic in the complex plane with the cut $[-1,1]$; also, observe that the integral over μ of $[g(\nu,\mu) - g(\mu,\mu)]/(\nu - \mu)$ vanishes, so that $g(\nu,\mu)$ in the last equation may be replaced by $g(\mu,\mu)$.

The discrete eigenvalues are paired, and will be denoted as $\pm\nu_0, \pm\nu_1, \ldots, \pm\nu_J$, with $|\nu_0| > |\nu_1| > \ldots$. When $c = 1$, the eigenvalues $\pm\nu_0 \to \infty$; this degeneracy and the complications that arise when there are eigenvalues imbedded in the continuum $[-1,1]$ are discussed elsewhere.[4,34] For $\nu_j \notin [-1,1]$, the Dirac delta term in Eq. (35) makes no contribution and therefore the eigenfunctions associated with the discrete spectrum are well-behaved functions. The eigensolutions $\phi_{\pm\nu_0}(\mu)\exp(\mp z/\nu_0)$ characterize the behavior of the flux far from interfaces and localized sources. For $c < 1$, the eigenvalues are real and ν_0 is the "transport-corrected" diffusion length which reduces for $c \to 1$ to the customary diffusion length $(h_0h_1)^{-1/2}$; when $c > 1$, ν_0 is purely imaginary and $|\nu_0|^{-2}$ represents the material buckling of the multiplying medium.[1,3,4]

Besides the discrete eigenvalues, there is a continuous spectrum $-1 \leq \nu \leq 1$; to every value of ν there corresponds a singular eigenfunction given by Eq. (35). In this case, the normalization condition provides the value of $\lambda(\nu)$ as the average of the analytical continuations of $\Lambda(\nu)$ as the cut $[-1,1]$ is approached from above and below.[4,34]

The set of eigenfunctions can be used to expand a broad class of functions of μ over the interval $[-1,1]$; the class of admissible functions for which completeness can be shown includes even $\delta(\mu - \mu_0)$ (Ref. 4). The eigenfunctions obey an orthogonality relation of the form

$$(\phi_\nu,\phi_{\nu'}) = \delta(\nu - \nu')N(\nu) , \quad (40)$$

where the inner product is

$$(f,g) = \int_{-1}^{1} f(\mu)g(\mu)\mu d\mu \quad (41)$$

and where the Dirac delta must be viewed as a Kronecker delta if one or both of the eigenvalues are discrete. The normalization function $N(\nu)$ is[4,34]

$$N(\nu) = \nu\left\{\lambda^2(\nu) + \left[\frac{1}{2}\pi c\nu g(\nu,\nu)\right]^2\right\} , \quad -1 \leq \nu \leq 1 ,$$

$$= \frac{1}{2} c\nu^2 g(\nu,\nu) d\Lambda(z)/dz\Big|_{z=\nu} , \qquad \nu = \pm\nu_j .$$

The solution of the transport equation follows by expanding the angular flux in terms of the eigenfunctions as

$$\psi(z,\mu) = \int_\sigma A(\nu)\phi_\nu(\mu)\exp(-z/\nu)d\nu + \psi_p(z,\mu) . \quad (42)$$

Here $\psi_p(z,\mu)$ is the particular solution that accounts for the effects of a spatially distributed source. The integral over the entire spectrum σ is equal to an integral on $[-1,1]$ plus a sum of the contributions from the points $\pm\nu_j$. The coefficients $A(\nu)$ of the expansion are calculated by applying orthogonality relations. For example, if the flux is known for $-1 \leq \mu \leq 1$ at a particular z within a homogeneous medium, then from Eqs. (40) and (42) we have

$$A(\nu)N(\nu)\exp(-z/\nu) = (\phi_\nu, \psi - \psi_p) , \quad \nu \in \sigma . \quad (43)$$

For realistic problems, one has to use more complicated orthogonality relations. The half-range biorthogonality relation over $0 \leq \mu \leq 1$ is applied when the incoming angular flux is known (as in the case of a vacuum boundary).[34] To treat full-range interface conditions between different media, orthogonality relation (40) must be supplemented with full-range equations involving eigenfunctions of both media.[34,38,39]

II.B. Spherical Harmonics Method

The idea behind this method is to separate the spatial and angular dependence of the flux by expanding the solution of the transport equation in terms of a complete set of angular basis functions (the spherical harmonics $\{Y_k^l\}$) (Refs. 3, 40, 41, and

[37]E. İNÖNÜ, *J. Math. Phys.*, **11**, 568 (1970).

[38]N. J. McCORMICK, *Nucl. Sci. Eng.*, **37**, 243 (1969).

[39]G. W. ECCLESTON and N. J. McCORMICK, *J. Nucl. Energy*, **24**, 23 (1970).

[40]W. KOFINK, *Nucl. Sci. Eng.*, **6**, 475 (1959).

[41]E. M. GELBARD, "Spherical Harmonics Methods: P_L and Double-P_L Approximations," *Computing Methods in Reactor Physics*, p. 267, H. GREENSPAN, C. N. KELBER, and D. OKRENT, Eds., Gordon and Breach, Science Publishers Ltd., New York (1968).

42). The resulting set of equations separates into an infinite set of coupled differential equations; in practice, approximate solutions are constructed by considering expansions on a finite subset of spherical harmonics. Within the context of approximation theory discussed in Sec. I.C, the spherical harmonics (SH) approximation of order N can be viewed as the projection method of Eq. (27) obtained with the subspace $\overline{\mathscr{E}}_N$ of functions spanned by $\{Y_k^l;\ |l| \leqslant k,\ k \leqslant N\}$.

The SH method may be written in operator notation as

$$PB\psi = PS \ . \tag{44}$$

Here $\psi \in \overline{\mathscr{E}}_N$ and P is the orthogonal projection on $\overline{\mathscr{E}}_N$ given by

$$P = \sum_{k \leqslant N} Q_k \ ,$$

where Q_k is given in Eq. (5). Equation (44) is a system of linear, coupled, first-order differential equations for the expansion coefficients $\psi_k^l(\boldsymbol{r})$ of the approximate solution ψ. These equations can be solved numerically by a finite difference approximation[41,43] or by the finite element method.[44]

In plane geometry, the only case we shall examine, the equations are amenable to analytical solution and the SH method becomes the Legendre polynomial or P_N method. As might be expected, this solution is closely related to that of the singular eigenfunction expansion method. For the sake of simplicity, we consider only the case of azimuthal symmetry, for which the angular flux depends only on z and μ. Then the approximate solution on $\overline{\mathscr{E}}_N$ may be written as

$$\psi(z,\mu) = \sum_{k \leqslant N} \frac{(2n+1)}{2} \psi_n(z) P_n(\mu) \tag{45}$$

and the projection P reduces to

$$P\psi = \sum_{n \leqslant N} \frac{2}{2n+1} P_n(\mu) \int_{-1}^{1} P_n(\mu')\psi(z,\mu')d\mu' \ .$$

Using these results, and the recursion relation for Legendre polynomials, Eq. (44) yields the P_N system of first-order differential equations

$$\mathbf{B}\boldsymbol{\psi} = \boldsymbol{S} \ . \tag{46}$$

Here $\boldsymbol{\psi}(z) = (\psi_n)$ is the vector of $N+1$ components $\psi_n(z)$, $n = 0$ to N, $\boldsymbol{S}(z) = (S_n)$, and $\mathbf{B} = (B_{nm})$ is a symmetric tridiagonal matrix operator with nonzero elements

$$B_{nn} = h_n = (2n+1)(1 - cf_n)$$

and

$$B_{n,n+1} = (n+1)\partial_z \ .$$

The solution of the system of Eqs. (46) can be written as a particular solution $\boldsymbol{\psi}_p$ plus a homogeneous solution. The latter is a linear combination of the $N+1$ linearly independent solutions of the homogeneous matrix equation

$$\mathbf{B}\boldsymbol{\psi} = 0 \ . \tag{47}$$

A solution of this equation is derived in the standard way; we substitute $g(\nu)\exp(-z/\nu)$ and obtain the equation

$$\mathbf{B}(\nu)\boldsymbol{g}(\nu) = 0 \ , \tag{48}$$

where $\mathbf{B}(\nu)$ is the matrix obtained from $\mathbf{B}$ by replacing ∂_z with $-1/\nu$. The condition for a nontrivial solution of this equation is that ν be a root of the characteristic equation $|\mathbf{B}(\nu)| = 0$. Comparison of this determinant with that of Eq. (38) shows that

$$|\mathbf{B}(\nu)| = \nu^{-(N+1)}(N+1)!\,g_{N+1}(\nu) \ , \tag{49}$$

which implies that the characteristic roots of Eq. (48) are the nonzero solutions of

$$g_{N+1}(\nu) = 0 \ . \tag{50}$$

For N even, the odd polynomial $g_{N+1}(\nu)$ has a root $\nu = 0$ and therefore Eq. (47) has only N linearly independent solutions. This is one indication that the P_{N+1} method for odd N may give inferior results to those obtained from the (odd-order) P_N approximation, and indeed this has generally been observed in P_N calculations; hence we consider only odd N approximations.

For odd N, the even polynomial $g_{n+1}(\nu)$ has $(N+1)/2$ pairs of roots denoted as $\pm\nu_j$, $j = 0$ to $(N-1)/2$, where $|\nu_0| > |\nu_1| > |\nu_2|$, etc. For $c < 1$, all these zeros are real and finite, while for $c = 1$ the values of $\pm\nu_0$ coalesce at infinity. When $c > 1$, the root ν_0 is imaginary and $|\nu_0|^{-2}$ again represents the material buckling of the multiplying medium.[1,3,4]

To calculate the eigenvectors $\boldsymbol{g}(\nu_j) = [g_n(\nu_j)]$, we adopt the normalization condition $g_0(\nu_j) = 1$. Then, comparison of Eq. (48) with recursion relation (37) shows that $g_n(\nu_j)$ is the value of the $g_n(\nu)$ polynomial at $\nu = \nu_j$. (This explains the notation selected for $\boldsymbol{g}$.)

Finally, the general solution to Eq. (46) may be written as

$$\boldsymbol{\psi}(z) = \int_{\sigma_N} A(\nu)\boldsymbol{g}(\nu)\exp(-z/\nu)d\nu + \boldsymbol{\psi}_p(z) \ ,$$

where the integral over σ_N denotes the sum over the set $\sigma_N = \{\pm\nu_j,\ j = 0 \text{ to } (N-1)/2\}$ and the $A(\nu)$ are the expansion coefficients. Use of this result in

[42]W. KOFINK, *Developments in Transport Theory*, p. 149, E. INÖNÜ and P. F. ZWEIFEL, Eds., Academic Press Inc., New York (1967).

[43]B. SIGG, *Nucl. Sci. Eng.*, **57**, 277 (1975).

[44]R. N. BLOMQUIST and E. E. LEWIS, *Nucl. Sci. Eng.*, **73**, 125 (1980).

Eq. (45) leads to the P_N solution to the transport equation

$$\psi(z,\mu) = \int_{\sigma_N} A(\nu)\phi_\nu^N(\mu)\exp(-z/\nu)d\nu + \psi_p(z,\mu) \ . \tag{51}$$

Here we have defined $\phi_\nu^N(\mu)$ as the Legendre expansion of order N,

$$\phi_\nu^N(\mu) = \sum_{n\leq N} \frac{2n+1}{2} g_n(\nu)P_n(\mu) \ , \quad \nu \in \sigma_N \ , \tag{52}$$

which implies that

$$g_n(\nu) = \int_{-1}^{1} P_n(\mu)\phi_\nu^N(\mu)d\mu \ , \quad \nu \in \sigma_N \ .$$

The similarity between the singular eigenfunction expansion (42) and the P_N expansion (51) is not surprising. For sufficiently large N, the first few pairs $\pm\nu_0, \ldots, \nu_J$ in σ_N approximate the discrete eigenvalues from Eq. (39), while the remaining pairs are in the interval $[-1,1]$. As N increases, the pairs $\pm\nu_j$, $j > J$, fill this interval even more densely until, in the limit, the whole interval $[-1,1]$ is reproduced so that $\sigma_N \to \sigma$.

In the sense of this limit, let $\nu_N \to \nu$ for $\nu_N \in \sigma_N$; then Eqs. (34) and (52) show that $\phi_{\nu_N}^N$ converges to ϕ_ν (in the L_2 norm) as[45]

$$\int_{-1}^{1} |\phi_{\nu_N}^N - \phi_\nu|^2 d\mu \to 0 \ .$$

It should be pointed out that in the classical introduction to the P_N method[3,4] the P_N equations are obtained by expanding $\psi(z,\mu)$ in terms of Legendre polynomials [as in Eq. (45) with $N \to \infty$]. Then, an infinite set of coupled differential equations for the $\psi_n(z)$ is obtained by multiplying the transport equation by $P_m(\mu)$ and integrating over $(-1,1)$; the set is truncated with the condition

$$d\psi_{N+1}(z)/dz = 0 \tag{53}$$

to recover Eq. (46).

We now examine two variations of the spherical-harmonics approximation in plane geometry, the "asymptotic P_N" and the "double P_N" methods. The essential feature of the asymptotic P_N method, abbreviated as AP_N, is to ensure that the asymptotic eigenvalues $\pm\nu_0$ equal those from the singular eigenfunction method (which can be viewed as a P_∞ method). In one variation of the AP_N method, the exact ν_0 is obtained directly as the largest root of $\Lambda(\nu)$ in Eq. (39), while the remaining eigenvalues ν_j, $j \geq 1$, are obtained as the nonasymptotic values from Eq. (50) (Ref. 46). In an earlier approach to the AP_N method, however, the entire set of eigenvalues were obtained from the determinant[47,48]

$$\begin{vmatrix} h_0\nu & 1 & 0 & . & . & . & 0 \\ 1 & h_1\nu & 2 & 0 & . & . & 0 \\ 0 & 2 & h_2\nu & 3 & 0 & . & 0 \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & 0 & [N+(N+1)\alpha_N] & & h_N\nu \end{vmatrix} = 0 \ ,$$

rather than from Eq. (50). The largest root ν_0 coincides with the exact one with the selection of the α_N such that $\alpha_N = g_{N+1}(\nu)/g_{N-1}(\nu)$; such an α_N corresponds to a truncation condition of

$$\psi_{N+1}(z) = \alpha_N\psi_{N-1}(z) \ ,$$

rather than Eq. (53).

For locations far from interfaces and localized sources, where the flux is nearly asymptotic, the AP_N method is superior to the corresponding P_N approximations; however, the AP_N method gives worse results when the flux is far from asymptotic.

The essential idea of the double $P_N(DP_N)$ method, sometimes referred to as Yvon's method, is to use a separate Legendre polynomial expansion over each half range of μ (Refs. 3, 4, and 6). Near strong discontinuities in the material properties, this representation allows one to account for a possible discontinuity at $\mu = 0$ in the angular flux. Even with a few terms in the approximation, such an expansion generally provides a good fit to a rapidly varying angular flux.

The DP_N equations are obtained by applying the projection technique on the space of functions spanned by $\{P_n^\pm(\mu), n \leq N\}$, for

$$P_n^\pm(\mu) = \begin{cases} P_n(2\mu \mp 1) \ , & \mu \gtrless 0 \ , \\ 0 \ , & \text{otherwise} \ . \end{cases}$$

The corresponding expansion for the angular flux is[6]

$$\psi(z,\mu) = \sum_{n\leq N} (2n+1)[\psi_n^+(z)P_n^+(\mu) + \psi_n^-(z)P_n^-(\mu)] \ .$$

Then Eq. (44) yields $2(N+1)$ coupled equations instead of the $(N+1)$ equations in the normal P_N method. The equations for $\psi_n^+(z)$ and $\psi_n^-(z)$ are coupled through the scattering term of the transport

[45]T. F. NONNENMACHER, *Developments in Transport Theory*, p. 343, E. İNÖNÜ and P. F. ZWEIFEL, Eds., Academic Press Inc., New York (1967).

[46]K. GANGULY and A. SENGUPTA, *Nucl. Sci. Eng.*, **74**, 1 (1980).

[47]G. C. POMRANING, *Nukleonik*, **6**, 348 (1964).

[48]G. C. POMRANING, *Nucl. Sci. Eng.*, **22**, 328 (1965).

equation, and therefore the solution of the DP_N equations generally involves about the same amount of work as for the P_{2N+1} equations.

Let us now briefly consider the boundary conditions to be used with these methods. A natural set of boundary conditions, the so-called "moment boundary conditions," follows by projecting the exact boundary conditions onto the set of Legendre polynomials used in the expansion. By this procedure the jump condition in Eq. (8) yields the $(N + 1)$ interface equations

$$\psi_n(z_0^+) - \psi_n(z_0^-) = \int_{-1}^{1} P_n(\mu) S_s(\mu) \mu^{-1} d\mu \ , \qquad n = 0 \text{ to } N \ ,$$

for the P_N and AP_N methods, where the $S_s(\mu)$ accounts for any localized source at z_0. Similarly, the moment conditions for an external boundary on the left side z_0 of the body are

$$\int_0^1 P_n(\mu)\psi(z_0,\mu)d\mu = \int_0^1 P_n(\mu)\psi_-(z_0,\mu)d\mu \ , \qquad n = 1, 3, \ldots, N \ .$$

These boundary conditions also are known as the Marshak conditions. The equation with $n = 1$ ensures, as in diffusion theory, continuity of the incoming neutron current; the choice of the remaining $(N - 1)/2$ odd moments for the remaining conditions admittedly is somewhat arbitrary.[3]

A second procedure for obtaining boundary conditions for the P_N methods is to precisely fit the exact boundary conditions at the $(N + 1)$ discrete angles $\{\pm\mu_k, k = 0 \text{ to } (N - 1)/2\}$; for an external surface, only half the directions are used, and the corresponding discrete-angle equations are called the Mark boundary conditions.[3] The angles $\pm\mu_k$ are paired to ensure rotational invariance, and normally are selected as roots of the equation $P_{N+1}(\mu) = 0$.

It is generally believed that the use of the moment conditions will lead to better accuracy for the solutions when N is low (perhaps $N \leqslant 5$ or 7, depending on c) and the discrete-angle conditions are preferable when N is larger.[3] For weakly absorbing media, however, the Marshak vacuum boundary conditions actually provide more accuracy[41] than the Mark vacuum boundary conditions for $1 \leqslant N \leqslant 19$.

At this point, a brief comparison of the ordinary, asymptotic, and double P_N methods is appropriate. At an interface, the ordinary P_N method is superior to the AP_N approach, but inferior to the DP_N; however, far from an interface, the P_N is better than the DP_N and inferior to the AP_N. A detailed comparison of the P_N and DP_N methods has been given by Williams.[6] In general, the DP_N and AP_N have not been widely adopted; of the three variants of P_N theory, the ordinary P_N method is the usual approach followed for numerical calculations.

II.C. Discrete Ordinates Methods

In this method, a finite set of N angular directions $\mathbf{\Omega}_m$ and associated weights w_m is used to define a quadrature formula on the sphere $\mathcal{S}_2$. Using this formula, the integral term of the transport equation simplifies to a linear combination of the angular fluxes $\psi_m(\boldsymbol{r}) = \psi(\boldsymbol{r},\mathbf{\Omega}_m)$. Then a set of N coupled differential equations for the $\psi_m(\boldsymbol{r})$ is obtained by specializing the transport equation to the set of directions $\{\mathbf{\Omega}_m, m = 1 \text{ to } N\}$.

The treatment of the spatial variable is based on a decomposition of the domain into a set of cells defined by a spatial mesh. For a given direction $\mathbf{\Omega}_m$, the angular fluxes $\psi_m(\boldsymbol{r})$ in a cell are described by a finite number of values, such as cell- or side-averaged fluxes. A cell-to-cell solution algorithm is characterized by

1. the formula used to calculate the emerging angular fluxes in terms of the entering angular fluxes and the volumetric source term
2. the formula used to update the source in terms of the cell angular fluxes.

There are two general philosophies for constructing such an algorithm. In the finite difference approximation, neutron balance over the cell constitutes the basic relation connecting the cell- and side-averaged fluxes; this equation must be supplemented with auxiliary relations, such as the diamond difference approximation. In the method of characteristics, the transport equation is integrated within a cell, along a set of neutron trajectories (or "characteristics"), to link the emerging angular fluxes to the entering angular fluxes and internal sources; the source term is obtained either by interpolation of the cell angular fluxes or from neutron balance arguments.

In the special case of plane geometry, there is also the possibility of solving the discrete ordinates equations in an analytical manner. Here we will first consider this "analytic discrete ordinates"[49] (or Wick-Chandrasekhar[2]) method and illustrate its connection with the singular eigenfunction and P_N methods. We discuss the more general finite difference approach and the method of characteristics afterwards.

II.C.1. Analytic Discrete Ordinates

In plane geometry, let $\{\mu_m, w_m, m = 1 \text{ to } N\}$ be the set of directions and associated weights defining

[49] J. MENNING, J. HALIN, C. LEPORI, and W. HÄLG, "Comparison of Analytical S_N and S_∞ Calculations with the Code ANISN," *Proc. IAEA Specialists Mtg. Methods of Neutron Transport Theory in Reactor Calculations*, Bologna, Italy, November 3-5, 1975, CONF-751152, International Atomic Energy Agency (1976).

the quadrature formula. Then for any function $f(\mu)$, we write

$$\int_{-1}^{1} f(\mu)d\mu \sim \sum_{m=1}^{N} f(\mu_m)w_m = \int_{S_N} f(\mu)d\mu \ ,$$

where the last integral symbol denotes the sum over the nodes in $S_N = \{\mu_m, m = 1 \text{ to } N\}$. This formula is now applied to the integral term in Eq. (7). Then the corresponding set of N coupled differential equations for the angular fluxes $\psi(z,\mu_m)$ can be written as

$$(\mu\partial_z + 1)\psi(z,\mu) = \frac{c}{2}\sum_{k\geq 0}(2k+1)f_k P_k(\mu) \times \int_{S_N} P_n(\mu')\psi(z,\mu')d\mu' + S(z,\mu) \ , \quad \mu \in S_N \ . \quad (54)$$

The solution of this system of equations is decomposed, as usual, into a particular solution plus a linear combination of homogeneous solutions. We proceed to calculate the homogeneous solution of the system of Eqs. (54). For a given $\mu \in S_N$, the corresponding homogeneous equation can be viewed as a linear differential equation for the angular flux $\psi(z,\mu)$, with a normalization condition on the right side. Thus, as in the singular eigenfunction method, we seek a solution of the form $\phi_\nu^N(\mu)\exp(-z/\nu)$ and obtain the corresponding Eq. (32) except that now the $g_k(\nu)$ in Eq. (34) is replaced by

$$g_k(\nu) = \int_{S_N} P_k(\mu)\phi_\nu^N(\mu)d\mu \ .$$

If we assume that $(\nu - \mu)$ is nonzero, then

$$\phi_\nu^N(\mu) = \frac{c}{2}\frac{\nu}{\nu-\mu}g(\nu,\mu) \ , \quad \mu \in S_N \ .$$

Within the limitation that

$$\frac{2k+1}{2}\int_{S_N} P_k(\mu)P_l(\mu)d\mu = \delta_{kl} \ , \quad k,l \leq K \ , \quad (55)$$

where K is the order of the anisotropic scattering, the calculation of the $g_k(\nu)$ is identical to that in the singular eigenfunction method. Hence, if we again select the normalization condition $g_0(\nu) = 1$, then $g_k(\nu)$ is the value of the k'th g polynomial for the eigenvalue ν.

The admissible values of ν are fixed by the normalization condition, which can be written as

$$\Lambda(\nu) = 0 \ , \quad (56)$$

where

$$\Lambda(\nu) = 1 - \frac{c}{2}\nu\int_{S_N}\frac{g(\nu,\mu)d\mu}{\nu-\mu} \ . \quad (57)$$

Except for the trivial case of $c = 0$, $\nu = \mu_m$ is not a root of Eq. (56) so we can multiply Eq. (57) by the product of factors $(\nu - \mu_m)$, $m = 1$ to N, and obtain a polynomial in ν of order N, which yields the set of N roots $\sigma_N = \{\nu_n, n = 1 \text{ to } N\}$. Then the solution for the angular flux can be written as in expansion (51). The coefficients of this expansion are calculated using discrete-angle boundary conditions at the set of directions S_N.

The quadrature formula should preserve all possible rotational symmetries. In plane geometry this implies that the μ_m must be symmetric about zero and the weights for two symmetric values must be identical. To avoid the ambiguities associated with the plane geometry transport equation for $\mu = 0$, only even N approximations are used in practice. Also, it is customary to use a Gauss-Legendre quadrature formula because it provides the best integration for polynomials.

To ensure that conditions (55) are satisfied, the order N of the approximation must be greater than the order K of the scattering law. Under these conditions it is possible to show that the spectrum σ_N of the analytic discrete ordinates method is identical to the spectrum for the P_{N-1} method. To prove this, we begin by rewriting Eq. (57) as

$$\Lambda(\nu) = 1 + c\nu\sum_{k\geq 0}(2k+1)f_k g_k(\nu)q_k(\nu) \ , \quad (58)$$

where we have used Eq. (33) and the definition

$$q_k(\nu) = \frac{1}{2}\int_{S_N}\frac{P_k(\mu)d\mu}{\nu-\mu} \ .$$

The function $q_k(\nu)$ can be written as a polynomial in ν, of degree $\leq (N-1)$, divided by the product of the N factors $(\mu_m - \nu)$, $m = 1$ to N. These functions obey the recursion relation

$$(k+1)q_{k+1}(\nu) - (2k+1)\nu q_k(\nu) + kq_{k-1}(\nu) = \delta_{k0} \ , \quad k \geq 0 \ , \quad (59)$$

where $q_{-1}(\nu) = 0$. A more convenient form than Eq. (58) can be derived by multiplying recursion relation (37) by $q_k(\nu)$ and subtracting the result from recursion relation (59) multiplied by $p_k(\mu)$. After summing over k from 0 to l, we obtain the Christoffel-Darboux formula

$$\Lambda(\nu) = (l+1)[g_l(\nu)q_{l+1}(\nu) - g_{l+1}(\nu)q_l(\nu)] \ , \quad (60)$$

valid for any $l \geq K$.

The proof that the spectra are identical is based on the use of this equation for $l = N$ and on the properties of the functions $q_k(\nu)$. We first observe that $q_N(\nu) = 0$ because the μ_m in the S_N Gauss-Legendre quadrature set are the roots of $P_N(\mu) = 0$. Also, for $k = N$, recursion relation (59) shows that $q_{N+1}(\nu)$ is proportional to $q_{N-1}(\nu)$. Repeated use of this recursion relation for $(N-1)$, $(N-2)$, . . . , 1 demonstrates that $q_0(\nu)$ equals $q_{N-1}(\nu)$ times a polynomial in ν of degree $(N-1)$. Then, since the degree

of the polynomial in the numerator of $q_0(\nu)$ is just $(N-1)$, it follows that $q_{N-1}(\nu)$ and $q_{N+1}(\nu)$ are of the form of a constant divided by the product of the N factors $(\mu_m - \nu)$, $m = 1$ to N. Finally, Eq. (60) for $l = N$ can be written in the form

$$\Lambda(\nu) \propto g_N(\nu) \Big/ \prod_{m=1}^{N} (\mu_m - \nu) \ ,$$

whereupon Eq. (56) for the analytic discrete ordinates method of order N is equivalent to the corresponding spherical harmonics Eq. (50) for the order $(N-1)$.

Both the S_N and the P_{N-1} approximations give the angular flux in the form of a linear combination of exponentials $\exp(-z/\nu_j)$ with the same arguments. Consequently, the two methods yield the same angular flux at the set of directions $\mu \in S_N$ provided that the discrete-angle boundary conditions are used in the P_{N-1} calculation.

II.C.2. Finite Difference Discrete Ordinates

The finite difference discrete ordinates approximation has been the subject of intense research, and the results are well documented in numerous reviews.[50-54] For this reason we will only illustrate the basic features of the method in some simple cases.

The quadrature set $\{\mathbf{\Omega}_m, w_m, m = 1 \text{ to } N, N \text{ even}\}$ must be selected so that it does not introduce an undesired directional bias. This is normally achieved by requiring that the set $S_N = \{\mathbf{\Omega}_m, m = 1 \text{ to } N\}$ be invariant for the main symmetries of the geometry. For example, in plane geometry where the orientation of the axis $\boldsymbol{e}_z$ is arbitrary, one selects the direction cosines $\mu_m = \mathbf{\Omega}_m \cdot \boldsymbol{e}_z$ such that S_N contains both μ_m and $-\mu_m$; rotational invariance and reflection arguments are invoked in more general geometries.[50] The corresponding weights w_m must obey the same symmetries and be positive; they may be selected by preserving moment conditions involving the angular integral or by associating an area on the unit sphere about each $\mathbf{\Omega}_m$.

II.C.2.a. Cartesian Coordinates

For a Cartesian geometry, a fixed coordinate system for $\mathbf{\Omega}$ can be used. Then the S_N approximation to the transport equation consists of the system of N differential equations

$$(\mathbf{\Omega} \cdot \nabla + \Sigma)\psi = q \ , \quad \mathbf{\Omega} \in S_N \ . \tag{61}$$

This set of equations is coupled through the emission density q, which is now approximated as

$$q = \int_{S_N} \Sigma_s(\boldsymbol{r}, \mathbf{\Omega}' \to \mathbf{\Omega}) \psi(\boldsymbol{r}, \mathbf{\Omega}') d\mathbf{\Omega}' + S \ , \tag{62}$$

where, as before, the integral on S_N stands for the weighted sum over the directions in S_N.

The solution of Eq. (61) is achieved by using a numerical approximation for the spatial derivative and by solving the resulting set of algebraic equations. To construct the approximation, we subdivide the spatial domain D into homogeneous rectangular parallelepiped zones D_i and integrate Eq. (61) over each zone. After use of the Gauss divergence formula, it follows that

$$V_i^{-1} \mathbf{\Omega} \cdot \int_{\partial D_i} \psi d\boldsymbol{A} + \Sigma_i \psi_i = q_i \ , \tag{63}$$

where V_i is the volume of zone i with total cross section Σ_i, ∂D_i is the surface of this zone, and the ψ_i and q_i are volume-averaged quantities. Next, the leakage through the surface is written in terms of surface-averaged fluxes as

$$V_i^{-1} \mathbf{\Omega} \cdot \int_{\partial D_i} \psi d\boldsymbol{A} = V_i^{-1} \sum_k \mu^k A_i^k (\psi_{i+}^k - \psi_{i-}^k) \ ,$$

where the summation is over the number of dimensions. Here the direction cosine $\mu^k = \mathbf{\Omega} \cdot \boldsymbol{e}_k$, where $\boldsymbol{e}_k$ is the unit vector in the direction of the k axis, A_i^k is the area of the surface with normal $\boldsymbol{e}_k$, and $(\psi_{i+}^k - \psi_{i-}^k)$ is the difference of the surface-averaged fluxes in the k direction.

Since there are more unknowns than equations, it is necessary to introduce a numerical approximation to relate the volume-averaged fluxes to the surface-averaged fluxes. The well-known "diamond difference" approximation gives the additional equations[52,53]

$$\psi_i = (\psi_{i+}^k + \psi_{i-}^k)/2 \ , \quad \text{all } k \ .$$

A few features of the numerical solution of the finite difference equations can be illustrated by considering the simple case of plane geometry.[55,56]

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[50] C. E. LEE, "The Discrete S_n Approximation to Transport Theory," LA-2595, Los Alamos National Laboratory (Mar. 1962).

[51] I. K. ABU-SHUMAYS, *Nucl. Sci. Eng.*, **64**, 299 (1977).

[52] B. G. CARLSON and K. D. LATHROP, "Transport Theory: The Method of Discrete Ordinates," *Computing Methods in Reactor Physics*, p.165, H. GREENSPAN, C. N. KELBER, and D. OKRENT, Eds., Gordon and Breach, Science Publishers Ltd., New York (1968).

[53] K. D. LATHROP, *React. Technol.*, **15**, 107 (1972).

[54] S. NAKAMURA, "New Formulation and Coarse-Mesh Acceleration for Two-Dimensional DS_N and P_N Methods," *Proc. Sem. Numerical Reactor Calculations*, Vienna, January 17-21, 1972, p. 51, International Atomic Energy Agency, Vienna (1973).

[55] R. E. ALCOUFFE, E. W. LARSEN, W. F. MILLER, and B. R. WIENKE, *Nucl. Sci. Eng.*, **71**, 111 (1979).

[56] E. W. LARSEN and W. F. MILLER, *Nucl. Sci. Eng.*, **73**, 76 (1980).

Then the explicit results for the final finite difference equation simplify to

$$\mu(z_{i+} - z_{i-})^{-1}(\psi_{i+} - \psi_{i-}) + \Sigma_i(\psi_{i+} + \psi_{i-})/2 = q_i \quad , \quad \mu \in S_N \quad , \qquad (64)$$

where the coordinate index ($k = 1$) has been dropped. The volume-averaged emission density q_i is calculated via Eq. (62) in terms of the right/left surface-averaged fluxes $\psi_{i\pm,m} = \psi_{i\pm}(\mu_m)$; in particular for isotropic scattering,

$$q_i = \Sigma_{s_i} \sum_{m=1}^{N} w_m(\psi_{i+,m} + \psi_{i-,m})/4 + (S_{i+} + S_{i-})/2 \quad , \quad \mu \in S_N \quad ,$$

where the diamond difference approximation has been used.

The system of Eqs. (64) may be solved in an iterative way by assuming in each "internal" iteration that the emission term q_i is known from the previous iteration. For a fixed direction $\mu \in S_N$, Eq. (64) is successfully solved in the direction of neutron propagation (such that if μ is negative then ψ_{i-} is computed in terms of ψ_{i+}, and vice versa); such a procedure ensures stability.[7] An iteration is begun at a spatial location having a prescribed angular flux (for example, a boundary at which the incoming flux is known), and is continued through the slab in the directions of the prescribed flux until the opposite boundary is encountered; at this point, the second boundary condition is used to calculate the starting values for the march through the slab in the opposite directions, and the procedure is continued until convergence is obtained.

A difficulty with the diamond difference approximation is that its use may produce negative fluxes. To circumvent this undesired feature, the diamond difference approximation is modified, whenever necessary, to ensure positivity.[53,57] For instance, one may set to zero the offensive negative flux, or one may use a weighted diamond difference formula,

$$\psi_i = \gamma\psi_{i+} + (1 - \gamma)\psi_{i-} \quad .$$

With $\gamma = 0.5$, the usual diamond scheme is recovered, while the "step approximation" defined by $\gamma = 1$ or 0 (according to whether $\mu > 0$ or < 0) gives a strictly positive scheme. An unpleasant side effect of such a positivity "fix" is that the accuracy of the numerical scheme is lower than that of the diamond difference approach,[7,26] which is of second order in the mesh size $(z_{i+} - z_{i-})$.

Alternate schemes to the standard diamond difference approximation include[55-59] the linear discontinuous approximation, the exponential method, the Hermite-Birkhoff interpolation, and approaches based on the method of characteristics, such as the step, linear, and quadratric[60] characteristic schemes. Most of these methods are superior to the diamond difference approximation in plane geometry.[55,56]

A desired feature of any numerical approximation to the transport equation is that the number of neutrons be conserved within each local volume, as in Eq. (24). This conservation has been built into the discrete ordinates approximation in Cartesian geometry because the discretization procedure was directly applied to the angle-dependent conservation equation (63) on each spatial zone.

II.C.2.b. Curvilinear Coordinates

Care must be exercised to ensure neutron conservation when constructing a discrete ordinates approximation to the transport equation in curvilinear geometries. (In these geometries, the direction vector $\boldsymbol{\Omega}$ is described in a local system of coordinates that depend on the spatial position.) Indeed, since the direction variables continuously change for a streaming neutron, extra terms involving derivatives with respect to the angular variable will appear in the leakage term $\boldsymbol{\Omega}\cdot\nabla$; hence, discretization may result in a nonconservative scheme. To avoid this, one has to apply the numerical approximation to the proper (i.e., conservative) form of the transport equation.

To write the conservative form of the equation in curvilinear coordinates, the leakage operator $\boldsymbol{\Omega}\cdot\nabla$, where $\boldsymbol{\Omega}$ is described in a fixed coordinate system, must be expressed in terms of the local system of coordinates (μ,χ), defined by the coordinate transformation $\mu = \mu(\boldsymbol{r},\boldsymbol{\Omega})$ and $\chi = \chi(\boldsymbol{r},\boldsymbol{\Omega})$. Then, in the curvilinear coordinate system $(\boldsymbol{r},\mu,\chi)$, the leakage operator becomes $\nabla_r\cdot\boldsymbol{\Omega} + R_{\boldsymbol{\Omega}}$, where ∇_r acts like ∇ but only on the spatial variable $\boldsymbol{r}$, while the angular redistribution operator, $R_{\boldsymbol{\Omega}}$, acts on the angular variables as

$$R_{\boldsymbol{\Omega}} = (\boldsymbol{\Omega}\cdot\nabla\mu)\partial_\mu + (\boldsymbol{\Omega}\cdot\nabla\chi)\partial_\chi - (\nabla_r\cdot\boldsymbol{\Omega}) \quad .$$

[57]B. G. CARLSON, *Nucl. Sci. Eng.*, **61**, 408 (1976).

[58]M. COURTOT, "Study of Some Numerical Schemes for Solving the Three-Dimensional Transport Equation," *Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems,* Munich, Germany, April 27-29, 1981, Vol. 1, p. 83, Kernforschungszentrum Karlsruhe (1981).

[59]E. H. BAREISS and K. L. DERSTINE, "An Automated Approach to Quantitative Error Analysis in Neutron Transport Calculations," ANL-76-59, Argonne National Laboratory (1976).

[60]D. V. GOPINATH, A. NATARAJAN, and V. SUNDARARAMAN, *Nucl. Sci. Eng.*, **75**, 181 (1980).

Note that although $\mathbf{\Omega}$ does not depend on the local spatial variables, the function $(\nabla_r \cdot \mathbf{\Omega})$ that arises from the interchange $\mathbf{\Omega} \cdot \nabla_r \Rightarrow \nabla_r \cdot \mathbf{\Omega} - (\nabla_r \cdot \mathbf{\Omega})$ does not necessarily vanish. This is because the divergence of the unit vectors in the local system of coordinates is not always zero. The explicit form for the angular redistribution operator for cylindrical, spherical, and toroidal geometries is given in Table I.

With the new form of the leakage operator, the transport equation appears as

$$(\nabla_r \cdot \mathbf{\Omega} + R_{\Omega} + \Sigma)\psi = q \ . \tag{65}$$

This equation is "conservative" in the sense that the integral over all angles of the angular redistribution term vanishes:

$$\int R_{\Omega} \psi d\mathbf{\Omega} = 0 \ , \tag{66}$$

so that Eq. (65) yields the usual conservation Eq. (24).

To obtain the S_N approximation in a curvilinear geometry, we select a quadrature set $\{w_m, \mathbf{\Omega}_m, m = 1 \text{ to } N, N \text{ even}\}$ and integrate transport Eq. (65) over the area w_m about $\mathbf{\Omega}_m$ on the unit directional sphere. The angular integral of the angular redistribution term can be done analytically, where the remaining terms are integrated with the usual S_N approximation

$$\int_{\Delta\Omega_m} f(\mathbf{\Omega}) d\mathbf{\Omega} \approx w_m f(\mathbf{\Omega}_m) \ ,$$

where the weight w_m equals the area of $\Delta\mathbf{\Omega}_m$. The resulting system of equations may be written as

$$[\nabla_r \cdot \mathbf{\Omega} + \bar{R} + \Sigma]\psi = q \ , \quad \mathbf{\Omega} \in S_N \ ,$$

where the average angular redistribution term is defined as

$$(\bar{R}\psi)(\boldsymbol{r}, \mathbf{\Omega}_m) = w_m^{-1} \int_{\Delta\Omega_m} R_{\Omega} \psi d\mathbf{\Omega} \ , \quad m = 1 \text{ to } N \ . \tag{67}$$

The finite difference approximation for the spatial leakage term $\nabla_r \cdot \mathbf{\Omega}\psi$ is done in the same way as for a Cartesian geometry. Thus, an integration over each zone D_i results in the following system of algebraic equations for the cell-averaged quantities:

$$V_i^{-1} \sum_k \mu^k [A_{i+}^k \psi_{i+}^k - A_{i-}^k \psi_{i-}^k] + (\bar{R}\psi)_i + \Sigma_i \psi_i = q_i \ , \quad \mathbf{\Omega} \in S_N \ . \tag{68}$$

Again the summation is over the number of dimensions and $\mu^k = \mathbf{\Omega} \cdot \boldsymbol{e}_k$, where $\boldsymbol{e}_k$ is the unit vector which corresponds to the k'th curvilinear coordinate; the $A_{i\pm}^k$ correspond to the outer/inner surface areas with normal $\boldsymbol{e}_k$.

For each geometry, the volume-averaged $(\bar{R}\psi)_i$ may be expressed in terms of the volume-averaged fluxes, $\psi_{i,m\pm}^l$, at the edges of the "angular cell" $\Delta\mathbf{\Omega}_m$. The index l, $l = 1$ or 2, indicates the angular coordinate corresponding to each derivative term $\partial\Omega_l$ in the operator R_{Ω}. The general expression one obtains is of the form

$$(\bar{R}\psi)_i = \sum_l [a_{i,m+}^l \psi_{i,m+}^l - a_{i,m-}^l \psi_{i,m-}^l] \ , \tag{69}$$

where the $a_{i,m\pm}^l$, which must be calculated for each geometry, depend on the spatial position i and may be shown to be proportional to the surface areas.[50]

TABLE I

Analytical Forms of the Angular Redistribution Operator

Geometry	Spatial Coordinates	Components of $\mathbf{\Omega}$ in Local Coordinate Systems[a]	Angular Redistribution Operator R_{Ω}
Cylindrical	r,ϕ,z	$(1-\mu^2)^{1/2}\cos\chi$, $(1-\mu^2)^{1/2}\sin\chi$, μ	$-\frac{(1-\mu)^{1/2}}{r}\partial_{\chi}\sin\chi$
Spherical	r,θ,ϕ	μ , $(1-\mu^2)^{1/2}\cos\chi$, $(1-\mu^2)^{1/2}\sin\chi$	$\frac{1}{r}\partial_{\mu}(1-\mu^2) - \frac{(1-\mu^2)^{1/2}}{r}\cot\theta\partial_{\chi}\sin\chi$
Toroidal[b]	$r,\theta,\mathbf{H}$	$(1-\mu^2)^{1/2}\cos\chi$, $(1-\mu^2)^{1/2}\sin\chi$, μ	$\frac{-\sin(\theta+\chi)}{\rho}\partial_{\mu}\mu(1-\mu^2)^{1/2} + \partial_{\chi}\left[\frac{1}{\rho}\frac{\mu^2}{(1-\mu^2)^{1/2}}\cos(\theta+\chi) - \frac{(1-\mu^2)^{1/2}}{r}\sin\chi\right]$

[a]Note that μ is the component of $\mathbf{\Omega}$ with respect to one of the three local coordinate axes, and χ is the projection of $\mathbf{\Omega}$ onto the plane defined by the other two axes.

[b]In terms of the major radius of the torus R, $\rho = R + r\sin\theta$ and $\mathbf{H}$ are the polar coordinates of the projection of the point onto the x-y plane, and $z = r\cos\theta$.

To solve the finite difference equations for the set of fluxes

$$\{\psi_{i,m}, \psi^k_{i\pm,m}, \psi_{i,m\pm}{}^l; \quad i = 1 \text{ to } I,\ m = 1 \text{ to } N,\ k = 1 \text{ to } 3,\ l = 1,2\} \ ,$$

it is necessary to add supplementary equations relating the volume-averaged fluxes $\psi_{i,m}$ to the surface-averaged fluxes $\psi^k_{i\pm,m}$ and to the volume-averaged fluxes on the edges of the angular cell $\psi_{i,m\pm}{}^l$. The diamond difference approximation is now generalized to

$$\begin{aligned} \psi_{i,m} &= (\psi^k_{i+,m} + \psi^k_{i-,m})/2 \ , \quad \text{all } k \\ &= (\psi_{i,m+}{}^l + \psi_{i,m-}{}^l)/2 \ , \quad \text{all } l \ . \end{aligned} \tag{70}$$

Moreover, additional supplementary equations are needed for boundary conditions on the angular dependence of the angular flux. These equations are usually constructed by considering the special directions for which the angular redistribution term vanishes, i.e., those directions along which the local neutron direction coordinates do not change with streaming.[50] (For example, for one-dimensional spherical geometry, the directions are the trajectories $\mu = \pm 1$ passing through the center of sphere, while for cylindrical coordinates the directions are the trajectories that intersect the axis, i.e., $\mu = \pm 1$ and $\chi = 0$ or π in the notation of Table I.) Another possibility to construct the boundary conditions on the angular dependence is to use a step function approximation such that the flux $\psi_{i,m}$ in the center of the angular cell is set equal to one of the edge values; the advantage is that fewer directions need be considered.[61]

We illustrate this formalism by considering the special case of the one-dimensional spherical geometry. Then the spatial dependence of the flux is only on r, so the zones can be defined by decomposing the sphere into homogeneous spherical shells $r_{i-} \leqslant r \leqslant r_{i+}$, $i = 1$ to I. Also, the summation over k in Eq. (68) may be suppressed. The only remaining complication is to calculate the angular redistribution term $(\bar{R}\psi)_i$. From the definition of Eq. (67) and the appropriate form of R_Ω given in Table I, we obtain

$$(\bar{R}\psi)(r,\mu_m) = \frac{2\pi}{w_m} \int_{\mu_{m-}}^{\mu_{m+}} \frac{1}{r} \times \partial_\mu [1-\mu^2)\psi] d\mu \ , \quad \mu_m \in S_N \ , \tag{71}$$

which depends on r only through the quantity (ψ/r). Next, the volume average in $(\bar{R}\psi)_i$ is obtained with the approximation

$$\left(\frac{\psi}{r}\right)_i \sim \psi_i \left(\frac{1}{r}\right)_i = \psi_i \left(\frac{A_{i+} - A_{i-}}{2V_i}\right) \ ,$$

while the μ integration is directly approximated by a linear combination of ψ_{m+} and ψ_{m-} with coefficients $\alpha_{m\pm}$. The final result is

$$(\bar{R}\psi)_i = \left(\frac{A_{i+} - A_{i-}}{V_i}\right) (\alpha_{m+}\psi_{i,m+} - \alpha_{m-}\psi_{i,m-}) \ , \tag{72}$$

and comparison with Eq. (69) shows that

$$a_{i,m\pm} = \left(\frac{A_{i+} - A_{i-}}{V_i}\right) \alpha_{m\pm} \ .$$

To obtain a conservative numerical scheme, one must constrain the $\alpha_{m\pm}$ values to satisfy the S_N counterpart of Eq. (66),

$$\sum_{m=1}^{N} w_m (\bar{R}\psi)_i = 0 \ ,$$

for any cell i. Combination of the last equation and Eq. (72) implies that

$$\sum_{m=1}^{N} w_m (\alpha_{m+}\psi_{i,m+} - \alpha_{m-}\psi_{i,m-}) = 0 \ .$$

Since this condition must be fulfilled for an arbitrary shape of the angular flux, and since $\psi_{i,(m+1)-} = \psi_{i,m+}$, we see that

$$\alpha_{N+} = \alpha_{1-} = 0 \ , \quad \alpha_{(m+1)-} = (w_m/w_{m+1})\alpha_{m+} \ , \quad m < N \ . \tag{73}$$

The remaining α_{m+} coefficients, $m < N$, are determined from a reference problem. It is customary to consider an infinite medium containing only a uniform isotropic source, so that the angular flux is uniform and isotropic. Then, conservation Eq. (24) implies that $\Sigma\psi = q$, so that the S_N transport Eq. (68) for spherical geometry reduces to

$$V_i^{-1}\mu[A_{i+} - A_{i-}]\psi + (\bar{R}\psi)_i = 0 \ , \quad \mu \in S_N \ .$$

With the aid of Eqs. (72) and (73), this equation gives a recursion relation for the α_{m+},

$$\alpha_{m+} = (w_{m-1}/w_m)\alpha_{(m-1)+} - \mu_m \ , \quad m > 1 \ , \tag{74}$$

with the starting condition

$$\alpha_{1+} = -\mu_1 \ . \tag{75}$$

The values of α_{m+} are all positive. For $m \leqslant (N/2)$, positivity may be seen directly from Eqs. (68) and (75); for $m > (N/2)$, it follows by considering the recursion relation for decreasing values of m, beginning now with the starting condition $\alpha_{(N-1)+} = \mu_N$.

Another way of looking at the calculation of

[61] K. D. LATHROP and F. W. BRINKLEY, "TWOTRAN-II: An Interfaced, Exportable Version of the TWOTRAN Code for Two-Dimensional Transport," LA-4848-MS, Los Alamos National Laboratory (1973).

the α_{m+} is to observe that a straightforward integration of Eq. (71) leads again to Eq. (72), but now with the $\alpha_{m\pm}$ defined by

$$\alpha_{m\pm} = \frac{\pi}{w_m}(1 - \mu_{m\pm}^2) \ , \quad m = 1 \text{ to } N \ .$$

Notice that the conservation conditions (73) hold automatically; also, since

$$\int_{\Delta\Omega_m} d\mathbf{\Omega} \sim w_m = 2\pi(\mu_{m+} - \mu_{m-}) \ ,$$

it follows that recursion relation (74) is maintained only if μ_m is selected as the average of μ_{m+} and μ_{m-}.

Any discussion of the S_N method would be incomplete without a consideration of its principal limitation, the so-called ray effect.[62] This effect arises because solution of the transport equation for only a discrete number of directions (or rays) leads to loss of invariance under infinitesimal rotations. Because of the S_N angular discretization, neutrons are propagated only along the rays. This fact implies that in multidimensional geometries the uncollided neutrons streaming from an isotropic source region, for example, are unable to reach zones that lie between rays emanating from the source. In practice the ray effect is aggravated for strongly absorbing media, as in shielding calculations. The ray effect is mitigated by increasing the number N of directions $\mathbf{\Omega}_m$, but this remedy requires increased computational effort and does not ensure a complete elimination of the problem.[63]

One possible fixup consists of introducing an artificial source distribution defined so that the S_N method becomes similar to the P_{N-1} approximation, which has rotational invariance.[64] This procedure leads to a better correction of the ray effect than increasing the order of the S_N approximation, but also involves heavy penalties in computation time.

A different way to remedy the ray effects is to abandon the discrete S_N angular representation in favor of an expansion on a set of angular functions. Instead of the computationally impractical P_N expansion, one may use Walsh functions[65] or piecewise polynomial expansions, as in the finite element method.[66] Nevertheless, the S_N method remains the technique most widely used for solution of the integrodifferential form of the transport equation.[61,67-69]

II.C.3. Method of Characteristics

In general, the diamond difference is a reasonable approximation when the scattering is important within the zones, and works well for reactor analysis problems. However, especially in deep-penetration shielding problems where neutron streaming effects are crucial, a large number of zones have to be used to obtain good accuracy, and calculations then become unreasonably expensive. This problem can be alleviated by using a different approximation that accounts for transport within the zones. In the method of characteristics,[26,70-73] such an approximation is obtained by analytical integration along the neutron trajectories (or "characteristics") in the directions $\mathbf{\Omega} \in S_N$, i.e., by using integral Eq. (18). The domain is divided into homogeneous cells, so that $\tau = \Sigma s$ in Eq. (18) and one assumes an analytic form for the spatial dependence of the volumetric emission density q, and thus the integration can be done analytically to give a closed-form relation linking the emerging and entering angular fluxes. In contrast to the finite difference approximation, the streaming term $\mathbf{\Omega}\cdot\nabla\psi$ of the transport equation

[62]K. D. LATHROP, *Nucl. Sci. Eng.*, **32**, 357 (1968).

[63]K. D. LATHROP, *Nucl. Sci. Eng.*, **45**, 255 (1971).

[64]W. F. MILLER and W. H. REED, *Nucl. Sci. Eng.*, **62**, 391 (1977).

[65]T. J. SEED and R. W. ALBRECHT, *Nucl. Sci. Eng.*, **60**, 337 (1976).

[66]L. L. BRIGGS, W. F. MILLER, and E. E. LEWIS, *Nucl. Sci. Eng.*, **57**, 205 (1975).

[67]K. D. LATHROP, "THREETRAN: A Program to Solve the Multigroup Discrete Ordinates Transport Equation in (x,y,z) Geometry," LA-6333-MS, Los Alamos National Laboratory (1976).

[68]W. W. ENGLE, "ANISN-ORNL, A One-Dimensional Discrete Ordinates Transport Code," CCC-254, Computer Technology Center, Union Carbide Corporation, Oak Ridge (1973).

[69]W. A. RHOADES and F. R. MYNATT, "DOT III, Two-Dimensional Discrete Ordinates Transport Code," ORNL-TM-4280, Oak Ridge National Laboratory (1973).

[70]J. R. ASKEW, "A Characteristic Formulation of the Neutron Transport Equation in Complicated Geometries," AEEW-M 1108, U.K. Atomic Energy Authority, Winfrith (1972).

[71]E. W. LARSEN and R. E. ALCOUFFE, "The Linear Characteristic Method for Spatially Discretizing the Discrete-Ordinates Equations in (X,Y)-Geometry," *Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems*, Munich, Germany, April 27-29, 1981, Vol. 1, p. 99, Kernforschungszentrum Karlsruhe (1981).

[72]R. E. ALCOUFFE and E. W. LARSEN, "A Review of Characteristic Methods Used to Solve the Linear Transport Equation," *Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems*, Munich, Germany, April 27-29, 1981, Vol. 1, p. 3, Kernforschungszentrum Karlsruhe (1981).

[73]M. D. BROUGH and C. T. CHUDLEY, "Characteristic Ray Solutions of the Transport Equation," *Advances in Nuclear Science and Technology*, Vol. 12, p. 1, J. LEWINS and M. BECKER, Eds., Plenum Press, New York (1980).

is treated exactly, so that the characteristic method is better suited for shielding problems.

Characteristic methods may be generally classified according to whether they use values of the angular flux at only a finite number of points on the cell surface, or they assume expansions for the angular flux over the cell faces.

In the first case, for each direction $\mathbf{\Omega} \in S_N$, one selects a finite number of characteristics and calculates the angular fluxes in direction $\mathbf{\Omega}$ at the points at which the characteristics intersect the cell boundaries.[70,74] Thus any existing flux is computed in terms of an entering flux and the source, which is typically assumed to be constant within the cell. To ensure neutron conservation, the source is evaluated by neutron balance within the cell: for each $\mathbf{\Omega} \in S_N$, this is done by distributing the volume of the cell between the characteristics that pass through the cell.

In such a general point-to-point approach, angular fluxes in different directions are calculated at different boundary locations. For a uniform spatial grid of homogeneous cells, however, it is possible to choose the angular directions so that the characteristics may be selected to intersect the corners (and possibly middle points) of the cell faces.[75,76] The advantage of the latter approach is that the exponential factors for the integration along the characteristics are the same for all cells comprised of the same material; the disadvantages are that the geometry must be divided into homogeneous squares (in two dimensions) or cuboids (in three dimensions), and that the set of discrete directions cannot be changed to improve the precision in the angular variable.

We now consider the class of characteristic methods that are based on the use of expansions for the angular flux over all cell faces. On each face k of the cell, the flux is approximated by

$$\psi^k(\mathbf{r},\mathbf{\Omega}) = \sum_j \psi_j^k(\mathbf{\Omega}) f_j^k(\mathbf{r}) \quad , \quad \mathbf{\Omega} \in S_N \quad , \qquad (76)$$

where the $f_j^k(\mathbf{r})$, $j = 1$ to J, are the expansion functions. The calculation of the expansion coefficients $\psi_j^k(\mathbf{\Omega})$ is done cell by cell. For a given cell and a fixed direction $\mathbf{\Omega}$, the integral equation gives the angular flux on an exiting face, $\psi^k(\mathbf{r},\mathbf{\Omega})$, in terms of the known flux for the entering face, $\psi^{\bar{k}}(\mathbf{r},\mathbf{\Omega})$, and the known source q.

The unknown expansion coefficients can be determined by either the collocation or projection method. In the collocation approach, a set of points $\{\mathbf{r}_i, i = 1 \text{ to } J\}$ on face k is used in integral Eq. (18), in conjunction with the expansions for the exiting and entering faces, to obtain the set of algebraic equations

$$\sum_j \psi_j^k(\mathbf{\Omega}) f_j^k(\mathbf{r}_i) = \sum_j \psi_j^{\bar{k}}(\mathbf{\Omega}) f_j^{\bar{k}}(\mathbf{r}_{ib}) \exp(-\tau_-) + \int_0^{s_b} q(\mathbf{r}_i - s\mathbf{\Omega},\mathbf{\Omega}) \exp(-\Sigma s) ds \quad ,$$

$$\mathbf{\Omega} \in S_N \quad . \qquad (77)$$

The point $\mathbf{r}_{ib} = \mathbf{r}_i - s_b\mathbf{\Omega}$ is on the entering face $\bar{k}$.

Such a method has been applied for the r-z geometry[77,78] by assuming a linear "continuous" expansion for the angular fluxes on the four cell faces. The expansion is continuous in the sense that the values of the fluxes on two adjacent faces are constrained to be the same at the common corner. These conditions of continuity reduce the number of unknown coefficients for a given $\mathbf{\Omega}$ from eight to four, and the fluxes are determined by selecting as collocation points the four corners of the cell. (Perhaps a different set of collocation points could improve the accuracy of the method, but such a set would certainly complicate the coding of the method.) The source term on the right side of Eq. (77) is analytically evaluated by assuming that the angular flux is linear along the characteristic,

$$\psi_i(\mathbf{r}_i - s\mathbf{\Omega},\mathbf{\Omega}) = \left(1 - \frac{s}{s_b}\right) \psi^k(\mathbf{r}_i,\mathbf{\Omega}) + \frac{s}{s_b} \psi^{\bar{k}}(\mathbf{r}_{ib},\mathbf{\Omega}) \quad ,$$

where $\psi^k(\mathbf{r}_i,\mathbf{\Omega})$ and $\psi^{\bar{k}}(\mathbf{r}_{ib},\mathbf{\Omega})$ are linearly interpolated from corner values. The fundamental disadvantage of this method is that neutron conservation is not guaranteed because the balance condition is not used, although use of linear interpolations results in an inherently positive scheme.

Another possibility to determine the unknown expansion coefficients is to use the projection method described in Sec. I.C. This technique has been applied by Larsen to x-y geometry by assuming a linear "discontinuous" approximation for the angular flux on each face k,[71,79]

$$\psi^k(\mathbf{r},\mathbf{\Omega}) = \psi_1^k(\mathbf{\Omega}) + \psi_2^k(\mathbf{\Omega}) \cdot (\boldsymbol{\rho} - \boldsymbol{\rho}_k) \quad , \qquad (78)$$

where $\boldsymbol{\rho}$ is the projection of $\mathbf{r}$ on the x-y plane and $\boldsymbol{\rho}_k$ denotes the midpoint of side k. Note that $\psi_1^k(\mathbf{\Omega})$ is the average angular flux on the side, while $\psi_2^k(\mathbf{\Omega})$

[74]M. J. HALSULL, "CACTUS—A Characteristic Solution to the Neutron Transport Equation in Complicated Geometries," AEEW-R 1291, U.K. Atomic Energy Authority, Winfrith (1980).

[75]M. R. WAGNER, D. A. SARGIS, and S. C. COHEN, *Nucl. Sci. Eng.*, **41**, 14 (1970).

[76]J. A. BUCHOLZ and C. G. PONCELET, *Nucl. Sci. Eng.*, **64**, 356 (1977).

[77]K. TAKEUCHI, *J. Nucl. Sci. Technol.*, **6**, 466 (1969) and **8**, 141 (1971).

[78]N. SASAMOTO and K. TAKEUCHI, *Nucl. Sci. Eng.*, **71**, 330 (1979).

[79]E. W. LARSEN, *Trans. Am. Nucl. Soc.*, **33**, 317 (1979).

is the gradient of the flux along the side (since $\boldsymbol{\rho}$ is a point constrained to be on the side). In this method, the angular flux within the cells is also taken to be linear, so that the source may be written as

$$q(\boldsymbol{r},\boldsymbol{\Omega}) = q_1(\boldsymbol{\Omega}) + \boldsymbol{q}_2(\boldsymbol{\Omega})\cdot(\boldsymbol{\rho} - \boldsymbol{\rho}_0) \ , \qquad (79)$$

where $\boldsymbol{\rho}_0$ is the center of the cell. Using this form for the source in integral Eq. (18) yields

$$\psi^k(\boldsymbol{r},\boldsymbol{\Omega}) = \bar{\psi^k}(\boldsymbol{r}_b,\boldsymbol{\Omega})\exp(-\tau_-) + \Sigma^{-1}\{[1-\exp(-\tau_b)] \times [q_1 + \boldsymbol{q}_2\cdot(\boldsymbol{\rho} - \boldsymbol{\rho}_0 - \Sigma^{-1}\boldsymbol{\Omega}_\rho)] + s_b\exp(-\tau_b)\boldsymbol{q}_2\cdot\boldsymbol{\Omega}_\rho\} \ ,$$

where $\boldsymbol{\Omega}_\rho$ is the projection of $\boldsymbol{\Omega}$ on the x-y plane; the incident angular flux $\bar{\psi^k}$ enters the cell at point $\boldsymbol{r}_b = \boldsymbol{r} - s_b\boldsymbol{\Omega}$.

The expansion coefficients $\psi_1^k(\boldsymbol{\Omega})$ and $\boldsymbol{\psi}_2^k(\boldsymbol{\Omega})$ are calculated by projection on the expansion functions. That is, we substitute Eq. (78) into the last equation and multiply the resulting expression first by unity and then by $(\boldsymbol{\rho} - \boldsymbol{\rho}_k)$. Then we integrate along the side to obtain explicit expressions for the expansion functions. To carry out the integration along a cell side, it is generally necessary to break up the domain of integration into two parts: one for which the particles enter through the opposite side, so that s_b is constant, and the other for which the particles enter through an adjacent side, so that s_b varies linearly.

To ensure neutron conservation, Larsen used the neutron balance equation when calculating the source. By substituting into Eq. (63) the expansions for the angular flux on the boundary and for the source in the cell, Eqs. (78) and (79), and the corresponding expansion for the angular flux in the cell, it follows that

$$\frac{\Omega_x}{l_x}\langle\psi_1^x(\boldsymbol{\Omega})\rangle + \frac{\Omega_y}{l_y}\langle\psi_1^y(\boldsymbol{\Omega})\rangle + \Sigma\psi_1(\boldsymbol{\Omega}) = q_1(\boldsymbol{\Omega}) \ , \quad \boldsymbol{\Omega}\in S_N \ ,$$

where

Ω_x = component of $\boldsymbol{\Omega}$ in the (horizontal) x direction

l_x = length of the horizontal side

$\langle\psi_1^x(\boldsymbol{\Omega})\rangle$ = difference between the expansion coefficients $\psi_1^k(\boldsymbol{\Omega})$ for the right and left vertical sides.

In this equation, $q_1(\boldsymbol{\Omega})$ is calculated in terms of $\psi_1(\boldsymbol{\Omega})$ using Eq. (62).

Calculation of the expansion coefficient $\boldsymbol{q}_2(\boldsymbol{\Omega})$ can be done by generalizing the idea underlying conservation Eq. (63). This is done by multiplying transport Eq. (61) by $(\boldsymbol{\rho} - \boldsymbol{\rho}_0)$ and integrating over the cell volume to obtain

$$12\frac{\Omega_x}{l_x}\overline{\psi_1^x(\boldsymbol{\Omega})} + \frac{\Omega_y}{l_y}\langle\psi_2^y(\boldsymbol{\Omega})\rangle l_x - 12\frac{\Omega_x}{l_x}\psi_1(\boldsymbol{\Omega}) + \Sigma\psi_{2x}(\boldsymbol{\Omega})l_x = q_{2x}(\boldsymbol{\Omega})l_x \ , \quad \boldsymbol{\Omega}\in S_N \ ,$$

and a similar equation for x interchanged with y; the $\overline{\psi_1^x(\boldsymbol{\Omega})}$ is the average value of $\psi_1^k(\boldsymbol{\Omega})$ for the two vertical sides of the cell. Although this procedure was used in the original application of the linear characteristic method, currently the calculation of the coefficients $\psi_2(\boldsymbol{\Omega})$ [and also $\boldsymbol{\psi}_2^k(\boldsymbol{\Omega})$] is done in a different way in order to improve computational efficiency.[71]

There are several conclusions that can be drawn from the work on characteristic methods. Since these methods account for uncollided neutron trajectories inside a cell, they are better suited for problems in which streaming dominates scattering. Characteristic methods that are based on linear expansions for the angular fluxes on the cell faces permit relatively larger cells than those required for the classical diamond difference approximation.[72] The use of quadratic or higher order expansions, which might reduce computational costs, certainly would require a positivity fix to ensure that the angular flux remains positive on the faces.

There is a trade-off in the scheme used to calculate the source within a cell. An inherently positive scheme can be obtained by calculating the source by using an interpolation scheme on the angular fluxes on the faces of the cell, although this approach does not preserve neutron conservation. In contrast, direct use of the balance equation when calculating the source ensures conservation, but may require a positivity fix. It seems that the second approach is better because forcing neutron conservation accelerates the convergence of the iterative scheme used for calculating the angular flux. As to the expansion for the source, use of a constant source is quite inefficient because it leads to small cells, so linear expansions like Eq. (79) offer computational advantages.

Work on characteristic methods is still under way. Besides the approximations discussed here, a hybrid method that combines the point-to-point characteristic method with the diamond difference approximation has been developed.[80,81]

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[80]W. L. FILIPPONE, S. WOOLF, and R. J. LAVIGNE, *Nucl. Sci. Eng.*, **77**, 119 (1981).

[81]W. L. FILIPPONE and S. WOOLF, "Application of the Method of Streaming Rays to Particle Transport in Complex Geometries," *Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems*, Munich, Germany, April 27-29, 1981, Vol. 1, p. 67, Kernforschungszentrum Karlsruhe (1981).

II.D. Finite Element Methods

The finite element method is an extension of the classical Rayleigh-Ritz-Galerkin technique for solving the variational formulation of a differential equation.[82] One of the method's most attractive features is that it uses a local expansion of the unknown function on piecewise polynomials that are zero over most of the domain. Each function enters the calculation at only a few nodes, and this results in a sparse system of algebraic equations. Furthermore, since each expansion function has a small support (i.e., the domain in which the function is nonzero is small), a good approximation for the unknown function on an arbitrary geometrical shape can be constructed by piecing together these "finite element" functions. Indeed, it is this versatility for complicated geometries that has made the finite element method popular in a variety of engineering disciplines.

The finite element method has been directly applied to the second-order transport equation for the even-parity component of the angular flux.[83] This flux $\psi^+(\boldsymbol{r},\boldsymbol{\Omega})$, along with the odd-parity component $\psi^-(\boldsymbol{r},\boldsymbol{\Omega})$, is defined as

$$\psi^{\pm}(\boldsymbol{r},\boldsymbol{\Omega}) = \frac{1}{2}\left[\psi(\boldsymbol{r},\boldsymbol{\Omega}) \pm \psi(\boldsymbol{r},-\boldsymbol{\Omega})\right] . \tag{80}$$

The even-parity transport equation has the advantage that it can be cast into a variational form, thus providing for a straightforward application of the finite element technique.

Although the ordinary transport equation for $\psi(\boldsymbol{r},\boldsymbol{\Omega})$ cannot be derived from a functional by a maximum or minimum principle, the finite element method can be applied to a variational form of the equation.[84,85] This alternate, weak formulation of the finite element method can be viewed as a Galerkin projection, as described in Sec. I.C. The difference, however, is that now some or all of the boundary conditions are directly incorporated.

The finite element procedure can be applied either to the spatial or angular variable, or simultaneously to both. The advantage of applying the technique to the spatial variable is that a good representation may be obtained for an arbitrary geometry. On the other hand, a finite element representation on the angular variable ameliorates the ray effects normally encountered in S_N solutions.

Here we first discuss the application of the finite element method to the ordinary transport equation, while treating simultaneously both the $\boldsymbol{r}$ and $\boldsymbol{\Omega}$ variables. Then we briefly analyze the differences that appear in the treatment of the even-parity transport equation.

II.D.1. Ordinary Form of the Transport Equation

When applying the Galerkin projective technique to transport Eq. (1), one looks for an approximate solution for the angular flux in a finite dimensional space E_N. This flux may be written as

$$\tilde{\psi}(\boldsymbol{r},\boldsymbol{\Omega}) \sim \sum_{i=1}^{N} \psi_i f_i(\boldsymbol{r},\boldsymbol{\Omega}) , \tag{81}$$

where the $\{f_i\}$ are a set of basis functions in E_N. Substitution of this approximation into the transport equation and projection of the resulting equation onto the expansion functions yields the set of algebraic equations

$$(f_i, B\tilde{\psi}) = S_i , \quad i = 1 \text{ to N} . \tag{82}$$

Here we have introduced the scalar product in phase space,

$$(f,g) = \int_X fg dx = \int_D \int_{4\pi} f(\boldsymbol{r},\boldsymbol{\Omega}) g(\boldsymbol{r},\boldsymbol{\Omega}) d\boldsymbol{r} d\boldsymbol{\Omega} ,$$

and we note that $S_i = (f_i, S)$.

The treatment of boundary conditions in the finite element method depends on whether these conditions can be incorporated into the equations or must be imposed on the expansion functions. The first are called "natural" boundary conditions, and the latter are called "essential." Since natural boundary conditions provide a convenient treatment in the finite element formulation, these conditions should be used whenever possible. Also, natural boundary conditions, which must include the inhomogeneous contribution ψ_0, will give rise to extra terms in the final equations.

For the ordinary form of the transport equation, all boundary conditions can be treated as natural conditions. If we assume that the expansion functions are continuous, we can use

$$f_i\boldsymbol{\Omega}\cdot\nabla\tilde{\psi} = -\tilde{\psi}\boldsymbol{\Omega}\cdot\nabla f_i + \boldsymbol{\Omega}\cdot\nabla(f_i\tilde{\psi}) , \quad f_i, \tilde{\psi} \in E_N , \tag{83}$$

to obtain the Green's formula

$$(f_i, B\tilde{\psi}) = (B^* f_i, \tilde{\psi}) + \langle f_i, \tilde{\psi}\rangle_+ - \langle f_i, \tilde{\psi}\rangle_- , \quad f_i, \tilde{\psi} \in E_N . \tag{84}$$

Here the adjoint operator B^* is defined as

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[82]G. STRANG and G. J. FIX, *An Analysis of the Finite Element Method*, Prentice-Hall Publishing Co., Inc., Englewood Cliffs, New Jersey (1973).

[83]S. KAPLAN and J. A. DAVIS, *Nucl. Sci. Eng.*, **28**, 166 (1967).

[84]S. UKAI, *J. Nucl. Sci. Technol.*, **9**, 366 (1972).

[85]T. OHNISHI, "Finite-Element Solution Technique for Neutron Transport Equation (F_N Approximation)," *Proc. Sem. Numerical Reactor Calculations*, Vienna, January 17-21, 1972, p. 629, International Atomic Energy Agency (1972).

$$B^* = -\boldsymbol{\Omega}\cdot\nabla + \Sigma - H$$

and the outgoing/incoming surface contributions are

$$\langle f,g\rangle_{\pm} = \pm \int_{\partial X_{\pm}} fg(\boldsymbol{\Omega}\cdot\boldsymbol{n})dx_{\pm}$$

$$= \pm \int_{\partial D}\int_{\pm 2\pi} f(\boldsymbol{r},\boldsymbol{\Omega})g(\boldsymbol{r},\boldsymbol{\Omega})(\boldsymbol{\Omega}\cdot\boldsymbol{n})dAd\boldsymbol{\Omega} \quad . \quad (85)$$

Formula (84) is now used to introduce boundary conditions into Eqs. (82) by replacing $\langle f_i,\tilde{\psi}\rangle_-$ with $\langle f_i,\tilde{\psi}_-\rangle_-$ where, with the notation of Eqs. (9) and (10), $\tilde{\psi}_- = \psi_0 + \beta\tilde{\psi}$. The resulting equations are

$$(B^*f_i,\tilde{\psi}) + \langle f_i,\tilde{\psi}\rangle_+ = S_i + \langle f_i,\tilde{\psi}_-\rangle_- \quad , \quad i = 1 \text{ to } N. \quad (86)$$

This equation constitutes the weak formulation of the finite element method of the transport equation. The formulation is "weak" in the sense that only the projections of the equation on the representation functions are satisfied. Indeed, if $\tilde{\psi}$ is a solution of Eq. (86), then with the aid of formula (84) this equation may be rewritten to obtain

$$(f_i, B\tilde{\psi} - S) + \langle f_i, \tilde{\psi} - \tilde{\psi}_-\rangle_- = 0 \quad . \quad (87)$$

This equation reduces to

$$(f_i, B\tilde{\psi} - S) = 0 \quad , \quad f_i \in E_N^0 \quad ,$$

where E_N^0 is the subspace of E_N containing the functions f_i that vanish on the incoming boundary ∂X_-. Furthermore, if the f_i become a complete set of functions as $N \to \infty$, then the last equation gives $B\tilde{\psi} = S$ almost everywhere, so that Eq. (87) implies that the boundary condition $\tilde{\psi} = \tilde{\psi}_-$ on ∂X_- is satisfied in the limit.

Use of expansion (81) in the set of Eqs. (86) leads to the matrix formulation of the finite element equations

$$\sum_{j=1}^{N} M_{ij}\psi_j = S_i + \langle f_i,\psi_0\rangle_- \quad . \quad (88)$$

The matrix elements M_{ij} are expressed in terms of volume and surface moments of the expansion function as

$$M_{ij} = (B^*f_i,f_j) + \langle f_i,f_j\rangle_+ - \langle f_i,\beta f_j\rangle_- \quad .$$

In Eq. (88) the inhomogeneous component of the boundary condition has been retained as part of the source term, while the homogeneous component has been included as a part of the matrix element.

Before discussing the calculation of the matrix elements, it is necessary to construct the expansion functions $f_i(\boldsymbol{r},\boldsymbol{\Omega})$. Two general approaches are possible: We can use a direct product of expansions in $\boldsymbol{r}$ and $\boldsymbol{\Omega}$ consisting of factorized functions which are a product of a spatial function and an angular function, or we can construct the expansion functions directly on the entire domain of $\boldsymbol{r}$ and $\boldsymbol{\Omega}$. The latter approach has been used for one-dimensional geometries, where only two variables are involved; more complicated geometries are treated with the factorized technique, which is discussed here for the case of a two-dimensional geometry.

To construct a finite element approximation on the spatial domain, we have to partition the domain into small homogeneous components and for each of them construct expansion functions with support on the subdomain. The shape of these geometrical elements should permit a good approximation to internal heterogeneities, such as fuel rods, and the contour of the external boundary. Rectangular elements,[86] and even general quadrilateral elements,[87-89] have been used, but here we consider only the more common triangular elements.

The expansion functions inside each triangular element are typically taken to be polynomials. For neutron transport theory, where only the flux need be continuous, Lagrange interpolation polynomials suffice[85]; Hermite interpolation polynomials, which also preserve continuity of the derivative of the flux, are not used. Only the simplest Lagrange approximation involving linear polynomials will be considered here.

A linear Lagrange interpolation polynomial inside the α'th triangle may be defined in terms of three linear basis functions, one for each vertex of the triangle. The function associated with vertex s is zero outside the triangle and is constructed so that

$$f_{s\alpha}(\boldsymbol{r}) = \begin{cases} 1 \ , & \text{vertex } s \\ 0 \ , & \text{other 2 vertices} \ . \end{cases} \quad (89)$$

Because the $f_{s\alpha}(\boldsymbol{r})$ is zero outside triangle α, it is discontinuous along the two sides intersecting vertex s. An expansion of the angular flux in terms of such functions therefore will be continuous within each triangle, but not necessarily along interfaces between

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[86]Y. MEDERBEL, "Résolution de l'Equation du Transport du 2ème Ordre par Application de la Méthode des Elément Finis sur l'Espace des Phases," Université de Paris Sud Thèse de 3ème Cycle (1977).

[87]P. LESAINT, *Rev. Française d'Automatique, Informatique et Recherche Operationnelle*, **R-2**, 67 (1974).

[88]J. GERIN-ROSE and P. LESAINT, *Int. J. Numer. Methods Eng.*, **10**, 171 (1976).

[89]M. MORDANT, "ZEPHYR, A Code for Solving Neutron Transport Problems on Irregular Meshes in Two Dimensional Geometries," *Proc. IAEA Specialists Mtg. Methods of Neutron Transport Theory in Reactor Calculations*, Bologna, Italy, November 3-5, 1975, CONF-751152, International Atomic Energy Agency (1976).

triangles. To achieve continuity, we sum the expansion functions for all triangles α with a common vertex s to obtain

$$f_s(\mathbf{r}) = \sum_{\alpha} f_{s\alpha}(\mathbf{r}) \ , \quad s = 1 \text{ to } N_s \ . \tag{90}$$

The set of $f_s(\mathbf{r})$ spans the appropriate subspace of functions that are continuous over all the N_s triangles and linear in each triangle.

The decomposition of the angular domain, which involves two variables, into subdomains depends on the coordinate system selected. With Cartesian coordinates Ω_x and Ω_y, the domain is the unit circle $\Omega_x^2 + \Omega_y^2 \leqslant 1$, and one can again use triangular elements to approximate the circumference of the domain.[85] On the other hand, use of polar coordinates with variables θ and ϕ gives a rectangular domain for which rectangular elements are more suitable.[90] The rectangular elements enable one to exactly match the perimeter of the rectangular domain, whereas the triangular elements can never fit exactly the unit circle. However, use of the variables (θ,ϕ) requires the evaluation of square roots and trigonometric functions to calculate the matrix elements M_{ij}, whereas this numerical complication is avoided with the use of the variables Ω_x and Ω_y.

The factorized finite element expansions that combine expansion functions $f_s(\mathbf{r})$ for space and $f_a(\mathbf{\Omega})$ for angle can be written as

$$f_i(\mathbf{r},\mathbf{\Omega}) = f_s(\mathbf{r}) f_a(\mathbf{\Omega}) \ , \quad i = 1 \text{ to } N \ ,$$

where $i \equiv (s,a)$ is a "two-dimensional" index linking the spatial index s, $s = 1$ to N_s, with the angular index a, $a = 1$ to N_a, and where $N = N_s N_a$. One advantage of such a factorized expansion function is that the calculation of the matrix elements is somewhat simplified by an uncoupling of integrals. For instance, for the volume element

$$(B^* f_i, f_j) = (-\mathbf{\Omega}\cdot\nabla f_i, f_j) + (\Sigma f_i, f_j) - (H f_i, f_j) \ , \tag{91}$$

we can write, with $j \equiv (s',a')$,

$$(\mathbf{\Omega}\cdot\nabla f_i, f_j) = \left[\int [\nabla f_s(\mathbf{r})] f_{s'}(\mathbf{r}) d\mathbf{r}\right] \cdot \left[\int \mathbf{\Omega} f_a(\mathbf{\Omega}) f_{a'}(\mathbf{\Omega}) d\mathbf{\Omega}\right] \ ,$$

$$(\Sigma f_i, f_j) = \left[\int \Sigma(\mathbf{r}) f_s(\mathbf{r}) f_{s'}(\mathbf{r}) d\mathbf{r}\right] \times \left[\int f_a(\mathbf{\Omega}) f_{a'}(\mathbf{\Omega}) d\mathbf{\Omega}\right] \ ,$$

and

$$(H f_i, f_j) = \int f_s(\mathbf{r}) f_{s'}(\mathbf{r}) \int f_{a'}(\mathbf{\Omega}) \times \int \Sigma_s(\mathbf{r},\mathbf{\Omega}'\cdot\mathbf{\Omega}) f_a(\mathbf{\Omega}') d\mathbf{r} d\mathbf{\Omega} d\mathbf{\Omega}' \ . \tag{92}$$

From the first two equations, we see that the elements can be obtained as products of spatial integrals and angular integrals; furthermore, if $\Sigma_s(\mathbf{r},\mathbf{\Omega}'\cdot\mathbf{\Omega})$ is expanded as in Eq. (3), then this factorization applies also to the third formula.

It is important to notice that since the representation functions $f_s(\mathbf{r})$ and $f_a(\mathbf{\Omega})$ vanish over much of the domain, the corresponding matrix elements likewise will vanish except when s and s' (and also a and a') are vertices in the same element; the only exception is the contribution from the scattering operator, which is totally coupled in angle. Consequently, the matrix is sparse with respect to the spatial variable.

Although the integrations in Eq. (92) can be evaluated analytically, they are usually carried out with a numerical integration scheme such as the Gauss quadrature. In such cases, each integral is decomposed into a set of integrations over the elements (triangle, rectangle, or whatever) and the contribution over a given element is calculated by mapping it into a reference element (an isosceles right triangle, a square, etc.) where the integration is carried out numerically. However, in order to ensure neutron conservation, the spatial gradient $\nabla f_s(\mathbf{r})$ is calculated analytically.

Convergence of the finite element method depends on the interpolation error, which generally varies as ρ_c^{k+1}/ρ_i, where ρ_c is the radius of the smallest circle circumscribing the element, ρ_i is the radius of the largest circle inscribed within the element, and k depends on the order of the polynomial approximation.[82,87,91] For triangular elements, for example, this means that elongated triangles result in poor convergence.

Until now, we have considered continuous finite element approximations, which, in principle, are required because the flux is a continuous function of the spatial variable. Use of discontinuous elements to approximate the angular variable, on the other hand, does not lead to any modifications to the formulas, and is advantageous in the treatment of boundaries (and, for example, to account for the possible discontinuity at $\mu = 0$ in a plane geometry). In the case of triangular elements, a discontinuous angular representation may be obtained from the

[90] W. F. MILLER, E. E. LEWIS, and E. C. ROSSOW, *Nucl. Sci. Eng.*, **52**, 12 (1973).

[91] P. JAMET, "Estimations d'Erreur pour des Eléments Finis Droits presque Dégénérés," DO 111, Commissariat à l'Energie Atomique, Limeil (Nov. 28, 1974).

direct use of basis functions (89) instead of the expanded functions (90).

For a given number of finite elements, discontinuous functions for the spatial variable may provide a better convergence,[92] even though they do not preserve continuity of flux at interfaces between elements. However, because of the spatial derivative operator ∇, special care should be taken when using discontinuous finite elements. To ensure the continuity of the angular flux as the number of elements N increases, one must include continuity at the interfaces as a natural boundary condition; that is, one must regard $\tilde{\psi}$ in Eq. (82) as if it were continuous. To obtain the correct form of the finite element equations, the same general procedure as before is followed. However, because the functions in E_N may be discontinuous, Eq. (83) is replaced by

$$f_i \boldsymbol{\Omega}\cdot\nabla\tilde{\psi} = -\tilde{\psi}\boldsymbol{\Omega}\cdot\nabla f_i + \boldsymbol{\Omega}\cdot\nabla(f_i\tilde{\psi}) - \langle\tilde{\psi}f_i\rangle\boldsymbol{\Omega}\cdot\boldsymbol{n}\delta_i(\boldsymbol{r}) \ , \quad f_i,\tilde{\psi}\in E_N \ . \tag{93}$$

In this expression, the derivatives are taken in the classical sense and the last contribution originates from the discontinuity of f_i; the $\delta_i(\boldsymbol{r})$ is the Dirac delta function on the perimeter of the support of f_i (i.e., of the i'th spatial element), and $\langle\tilde{\psi}f_i\rangle$ denotes the jump in the direction of the normal $\boldsymbol{n}$ to the perimeter. Use of Eq. (93) again yields Eq. (86) except that an extra term

$$T_i = -\iint \tilde{\psi}\langle f_i\rangle(\boldsymbol{\Omega}\cdot\boldsymbol{n})d\boldsymbol{\Omega}dl \tag{94}$$

must be added to the left side. The line integral on dl is performed along the perimeter of the i'th spatial element.

The specific form for T_i in Eq. (94) has been obtained by imposing the natural boundary condition of continuity of $\tilde{\psi}$ at the interfaces, so that $\langle\tilde{\psi}f_i\rangle = \tilde{\psi}f_a(\boldsymbol{\Omega})\langle f_s(\boldsymbol{r})\rangle$. To calculate the contribution of the integral T_i to the matrix M_{ij}, one must replace $\tilde{\psi}$ by its expansion in Eq. (81). Since this expansion is discontinuous, it is necessary to give a rule for calculating $\tilde{\psi}$ along the discontinuity; if the equations are solved according to the direction of neutron travel, then the known $\tilde{\psi}$ is used, corresponding to $\tilde{\psi}(\boldsymbol{r}-\epsilon\boldsymbol{\Omega},\boldsymbol{\Omega})$ for vanishing ϵ.

To construct the discontinuous spatial elements $f_s(\boldsymbol{r})$, one possibility is to use directly the basis functions (89). Another possibility is to use a function that vanishes outside of any two adjacent triangles, vanishes at the midpoint of all exterior sides, equals unity at the midpoint of the side common to the two triangles, and that is a linear function in each of the triangles.[82]

[92]W. R. MARTIN and J. J. DUDERSTADT, *Nucl. Sci. Eng.*, **62**, 371 (1977).

The finite element equations, as developed simultaneously in $\boldsymbol{r}$ and $\boldsymbol{\Omega}$, lead to an asymmetric matrix $\mathbf{M}$ that is not well suited for an iterative procedure. This means that the solution must be obtained by direct numerical inversion. At present this disadvantage overshadows the fact that this finite element method is less susceptible to ray effects and flux oscillations, that it leads to a simple treatment of all boundary conditions as natural conditions, and that it offers the possibility of using discontinuous approximations.[7]

As a possible compromise, a mixed scheme, consisting of a finite element approach for $\boldsymbol{r}$ and a discrete ordinates representation for $\boldsymbol{\Omega}$, leads to a set of algebraic equations which are amenable to solutions by an explicit technique.[89,93,94] Such a solution technique permits calculation of the flux at successive spatial locations following the direction of neutron travel. In this mixed scheme, boundary conditions cannot be treated as natural boundary conditions and must be incorporated as they arise. Also, since the incoming boundaries of an element depend on the neutron direction, special care has to be taken when devising the iterative procedure for sweeping the mesh.

II.D.2. Even-Parity Form of the Transport Equation

The even parity form of the neutron transport equation is derived by first writing the transport equation twice, for $\boldsymbol{\Omega}$ and $-\boldsymbol{\Omega}$, and adding and subtracting the equations to obtain

$$\boldsymbol{\Omega}\cdot\nabla\psi^{\mp} + (\Sigma - H^{\pm})\psi^{\pm} = S^{\pm} \ . \tag{95}$$

Here $\psi^{\pm}$ has been defined in Eq. (80), and $S^{\pm}$ is defined similarly. The operators $H^{\pm}$ are similar to the scattering operator H except that the corresponding kernels are

$$\Sigma_s^{\pm}(\boldsymbol{r},\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}) = \frac{1}{2}\left[\Sigma_s(\boldsymbol{r},\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega}) \pm \Sigma_s(\boldsymbol{r},-\boldsymbol{\Omega}'\cdot\boldsymbol{\Omega})\right] \ .$$

The even-parity form of the transport equation follows by solving the second equation of (95) for ψ^-,

$$\psi^- = K(S^- - \boldsymbol{\Omega}\cdot\nabla\psi^+) \ , \tag{96}$$

where $K = (\Sigma - H^-)^{-1}$; then substituting this result into the first equation, we obtain the even parity

[93]W. H. REED, T. R. HILL, F. W. BRINKLEY, and K. D. LATHROP, "TRIPLET: A Two-Dimensional, Multigroup, Triangular Mesh, Planar Geometry, Explicit Transport Code," LA-5428-MS, Los Alamos National Laboratory (1973).

[94]T. J. SEED, W. F. MILLER, and F. W. BRINKLEY, "TRIDENT: A Two-Dimensional Multigroup, Triangular Mesh Discrete Ordinates, Explicit Neutron Transport Code," LA-6735-M, Los Alamos National Laboratory (1977).

equation[83]

$$(-\mathbf{\Omega}\cdot\nabla K\mathbf{\Omega}\cdot\nabla + \Sigma - H^+)\psi^+ = S^+ - \mathbf{\Omega}\cdot\nabla KS^- \quad . \quad (97)$$

The operator K is calculated by writing H^- in terms of the orthogonal projection operators Q_k. This results in an equation like Eq. (4) except that the summation now is over only the odd terms. Then, using the properties of Q_k, it can be shown that

$$K = \Sigma^{-1}\left[1 + \sum_{k\ \text{odd}} \frac{\Sigma_{sk}}{(2k+1)(\Sigma - \Sigma_{sk})} Q_k\right] \quad , \quad (98)$$

provided that the medium is at least slightly absorbing.

The solution of Eq. (97) requires the evaluation of $S^{\pm}$, the even and odd components of the source. In a multigroup calculation, these sources depend on the corresponding angular fluxes $\psi^{\pm}$ and, although ψ^+ is the direct solution of Eq. (97), extra numerical effort is needed to obtain ψ^- using Eq. (96). This complication has been avoided by most researchers[66,90,92,95-99] who have considered only the special case of isotropic scattering and sources, where $K = \Sigma^{-1}$ and $S^- = 0$; then the even parity equation is

$$\left[-\mathbf{\Omega}\cdot\nabla\Sigma^{-1}\mathbf{\Omega}\cdot\nabla + \Sigma - (4\pi)^{-1}\Sigma_s \int d\mathbf{\Omega}\right]\psi^+ = S^+ \quad .$$

Knowledge of the resulting ψ^+ is sufficient to calculate the total flux ϕ that, in turn, gives any desired reaction rate.

It still remains to prescribe the interface and boundary conditions to be used with the second-order form (97) of the transport equation. When there are no surface sources, the angular flux is continuous at any interface and both ψ^+ and ψ^- are continuous. It is convenient to rewrite the boundary conditions in a more symmetric form valid for an arbitrary $\mathbf{\Omega}$. This can be done by introducing the sign function

$$s = -\frac{\mathbf{\Omega}\cdot\boldsymbol{n}}{|\mathbf{\Omega}\cdot\boldsymbol{n}|} \quad ,$$

so that the general boundary condition of Eqs. (9) and (10), $\psi = \psi_- = \psi_0 + \beta\psi$ on ∂X_-, now becomes

$$\psi(s\mathbf{\Omega}) = \psi_-(s\mathbf{\Omega}) \quad , \quad \text{on } \partial X \quad . \quad (99)$$

To write this equation in terms of the even and odd components of the angular flux, we first observe that

$$\psi(s\mathbf{\Omega}) = \psi^+(\mathbf{\Omega}) + s\psi^-(\mathbf{\Omega}) \quad .$$

For convenience, the albedo operator β of Eq. (10) also is extended to functions defined on the entire boundary ∂X that is comprised of all points in phase space $X = (\boldsymbol{r},\mathbf{\Omega})$ for which $\boldsymbol{r} \in \partial D$. The kernel $\beta(x' \to x)$, whose values are known for $\mathbf{\Omega}'\cdot\boldsymbol{n} > 0$ and $\mathbf{\Omega}\cdot\boldsymbol{n} < 0$, is now defined for arbitrary $\mathbf{\Omega}$ and $\mathbf{\Omega}'$ with the formulas

$$\beta(x' \to x) = 0 \quad , \quad (\mathbf{\Omega}'\cdot\boldsymbol{n}) \text{ and } (\mathbf{\Omega}\cdot\boldsymbol{n}) > 0 \quad ,$$

and

$$\beta(x' \to x) = \beta(R^-x' \to R^-x) \quad ,$$

where R^- is the operator that reverses the angular direction, $R^-x = R^-(\boldsymbol{r},\mathbf{\Omega}) = (\boldsymbol{r},-\mathbf{\Omega})$; then it can be shown that

$$(\beta\psi)(s\mathbf{\Omega}) = \beta(\psi^+ - s\psi^-) \quad .$$

Using this formalism, boundary condition (99) can be written as

$$(1-\beta)\psi^+ + (1+\beta)s\psi^- = \psi_0(s\mathbf{\Omega}) \quad , \quad \text{on } \partial X \quad , \quad (100)$$

and after accounting for Eq. (96), this gives the appropriate boundary condition in terms of ψ_+ for the even parity equation (97).

An early scheme for the solution of the even-parity form of the transport equation used an angle-space synthesis method closely related to the finite element approximation.[100] Just as with the ordinary form of the transport equation, the finite element approximation to the even-parity form is obtained with a Galerkin approximation. Use of an expansion like the one in Eq. (81) yields

$$(f_i,\mathbf{\Omega}\cdot\nabla\psi^-) + (f_i,[\Sigma - H^+]\psi^+) = (f_i,S^+) \quad ,$$

where ψ^- is defined in terms of ψ^+ via Eq. (96). As many of the interface and boundary conditions as possible should be incorporated as natural conditions in this equation. Again, for simplicity, we assume that the expansion functions are continuous, so that Eq. (83) (with $\tilde{\psi}$ now replaced by $\tilde{\psi}^-$) can be used to rewrite the contribution from the spatial leakage term as

$$(f_i,\mathbf{\Omega}\cdot\nabla\tilde{\psi}^-) = (\mathbf{\Omega}\cdot\nabla f_i, K\mathbf{\Omega}\cdot\nabla\tilde{\psi}^+) - (\mathbf{\Omega}\cdot\nabla f_i, KS^-) + \langle f_i,\tilde{\psi}^-\rangle \quad .$$

[95]W. F. MILLER, E. E. LEWIS, and E. C. ROSSOW, *Nucl. Sci. Eng.*, **51**, 148 (1973).

[96]J. PITKÄRANTA and P. SILVENNOINEN, *Nucl. Sci. Eng.*, **52**, 447 (1973).

[97]H. G. KAPER, G. K. LEAF, and A. J. LINDEMAN, "Applications of Finite Elements in Reactor Mathematics. Numerical Solution of the Neutron Transport Equation," ANL-8126, Argonne National Laboratory (1974).

[98]E. E. LEWIS, W. F. MILLER, and T. P. HENRY, *Nucl. Sci. Eng.*, **58**, 203 (1975).

[99]L. L. BRIGGS and E. E. LEWIS, *Nucl. Sci. Eng.*, **75**, 76 (1980).

[100]S. KAPLAN, J. A. DAVIS, and M. NATELSON, *Nucl. Sci. Eng.*, **28**, 364 (1967).

The total surface term

$$\langle f_i, \tilde{\psi}^- \rangle = \int_{\partial X} f_i \tilde{\psi}^- (\boldsymbol{\Omega} \cdot \boldsymbol{n}) dx$$

is now simplified with the help of interface or boundary conditions, as appropriate.[101]

When there are no surface sources, the interface conditions may be incorporated as natural conditions. Indeed, in this case, the angular flux ψ^- is continuous and therefore the surface term vanishes. We consider now the boundary conditions. If the operator $(1 + \beta)$ can be inverted, the surface term becomes

$$\langle f_i, \tilde{\psi}^- \rangle = \langle f_i, s(1 + \beta)^{-1} [\psi_0(s\boldsymbol{\Omega}) - (1 - \beta)\tilde{\psi}^+] \rangle \ .$$

Thus, any boundary condition can be incorporated as a natural boundary condition; in particular, for the case of $\beta = 0$ this includes a purely inhomogeneous boundary condition as, for example, for a nonreentrant boundary. In some situations of physical interest, however, the operator $(1 + \beta)$ cannot be inverted; such is the case of isotropic or specular reflection defined in Eq. (11) when $\beta(\boldsymbol{r}) = 1$.

Here we show that the often-used specular reflection boundary condition with unit albedo can be treated as an essential condition. Since for this condition the square of the albedo operator is unity ($\beta^2 = 1$), application of the operators $(1 \mp \beta)$ to Eq. (100) yields

$$\psi^+ = \beta\psi^+ + \frac{1}{2}(1 - \beta)\psi_0(s\boldsymbol{\Omega})$$

and

$$\psi^- = \beta\psi^- + \frac{1}{2} s(1 + \beta)\psi_0(s\boldsymbol{\Omega}) \ ,$$

where the anticommutation relation $\beta s = -s\beta$ has been used. The second equation can be used to obtain

$$\langle f_i, \tilde{\psi}^- \rangle = \langle f_i, \beta\tilde{\psi}^- \rangle + \left\langle f_i, \frac{1}{2} s(1 + \beta)\psi_0(s\boldsymbol{\Omega}) \right\rangle \ . \qquad (101)$$

To eliminate the spatial derivatives on the boundary that arise in the first term on the right side, we introduce the adjoint albedo operator β^* via the identity

$$\langle f_i, \beta\tilde{\psi}^- \rangle = \langle \beta^* f_i, \tilde{\psi}^- \rangle \ .$$

We then observe that if we construct the expansion functions so that, for any function g in E_N,

$$\langle (1 + \beta^*) f_i, g \rangle = 0 \ , \qquad (102)$$

then Eq. (101) simplifies to

$$\langle f_i, \tilde{\psi}^- \rangle = \left\langle f_i, \frac{1}{4} s(1 + \beta)\psi_0(s\boldsymbol{\Omega}) \right\rangle \ .$$

For specular reflection, for which $\beta^* = -\beta$, condition (102) reduces to the essential boundary conditions

$$f_i(\boldsymbol{r}, \boldsymbol{\Omega}) = f_i[\boldsymbol{r}, \boldsymbol{\Omega} - 2(\boldsymbol{\Omega} \cdot \boldsymbol{n})\boldsymbol{\Omega}] \ , \quad \boldsymbol{r} \in \partial D \ .$$

In other words, the expansion functions f_i must satisfy the specular reflection condition.[97]

As for the ordinary form of the transport equation, piecewise polynomials are used to construct the approximations in the space and angular domains. It should be mentioned, however, that spherical harmonics have been used as expansion functions over the angular domain, and this leads to a complete elimination of the ray effects.[44]

The application of the finite element method in both variables $\boldsymbol{r}$ and $\boldsymbol{\Omega}$ has two advantages when compared to the corresponding treatment of the ordinary, first-order form. First, since the operator in transport Eq. (97) is self-adjoint, the corresponding matrix $\mathbf{M}$ is symmetric and the equation is amenable to solution by iterative techniques.[86,97,102] The second advantage is that the domain of the angular variable for ψ^+ is halved, so that fewer angular finite elements are needed to obtain the same precision.

On the other hand, the frequently encountered specular reflection boundary condition cannot be treated as a natural condition, and therefore special expansion functions must be used for the even-order equation. An additional disadvantage of this equation arises from the fact that the even parity flux depends on the angular fluxes in the $\boldsymbol{\Omega}$ and $-\boldsymbol{\Omega}$ directions. Consequently, the resulting numerical method is implicit and cannot be solved iteratively by following the neutron trajectories.[97] Still other difficulties with the method are encountered in the treatment of tenuous media [see Eq. (98)] and in the incorporation of anisotropic scattering.

The finite element form of the even-order transport equation circumvents the nagging concerns with such troubles as the ray effect arising in the discrete ordinates method, alleviates flux oscillations, and offers a direct representation for complicated geometries. Nonetheless, the inherent limitations of this finite element method have made it unattractive compared to the highly developed discrete ordinates approach.[7,97] However, this may change

[101] H. G. KAPER, G. K. LEAF, and A. J. LINDEMAN, *J. Math. Anal. Appl.*, **50**, 42 (1975).

[102] Y. C. YUAN, E. E. LEWIS, and W. F. MILLER, "Iterative Solution Methods for Two-Dimensional Finite Element Approximations in Neutron Transport," *Proc. Conf. Computational Methods in Nuclear Engineering*, Charleston, South Carolina, April 15-17, 1975, CONF-750413, Vol. II, p. III-85, U.S. Energy Research and Development Administration (1975).

with the parallel processing available on vector computers. For example, it recently has been reported that a discretization of the even-parity form of the transport equation using discrete ordinates in angle and finite elements in space is superior to the conventional discrete ordinates approach in plane geometry.[103]

III. INTEGRAL EQUATION METHODS

The basic approach for the treatment of the integral form of the transport equation is to eliminate the angular dependence by projecting the equation onto the set of spherical harmonics, as in the P_N method. For a scattering law of finite order, the resulting system of integral equations for the angular moments of the flux is closed; this contrasts with the P_N approximation, which requires an extra assumption to close the set. Nevertheless, the solution of even a few coupled integral equations is a formidable task. Usually one considers the case of isotropic scattering and sources, for which there is only one integral equation.

In this section, three basic numerical methods [discrete integral transport (DIT), collocation, and collision probability (CP)] are described and compared for the isotropic scattering case. The DIT technique results from the use of a numerical quadrature formula, whereas the other two methods are obtained by using a finite expansion for the total flux. The collocation and CP methods follow by use of the collocation and projection techniques described in Sec. I.C.

Since the CP method is the most widely used of the three, the subsequent discussion is focused on this method.[104-108] First we describe the usual CP flat flux (i.e., piecewise constant) approximation in the one-dimensional and Cartesian x-y geometries. The flat flux approximation is well suited for systems with small dimensions. To make the CP method practical for optically large media, a generalized piecewise approximation can be constructed by using several expansion functions to provide a good representation for the gradient of the flux within a zone.

Following this, application of the CP method to problems with linearly anisotropic scattering and sources is discussed for the one-dimensional geometries. For these geometries, the neutron continuity equation allows for simplification of the system of integral equations for the flux and net current to a single integral equation for the flux.

In the special case of a homogeneous medium, a quasi-analytical method, the spatial spherical harmonics (SSH) method, results from use of a continuous multifunction expansion of the flux within the CP approach. This method and an equivalent method that deals with the Fourier transformed equation, the integral transform (IT) method, also are described for one-dimensional geometries with isotropic and linearly anisotropic scattering.

Finally, we discuss the interface current and transverse nodal methods. The philosophy behind these two techniques is to divide a large medium into subregions or nodes and to use a simplified model to describe the transport between nodes. A particular feature of the transverse nodal method is that integration over one or two of the spatial variables is used to reduce the problem to a set of coupled one-dimensional problems.

III.A. Elimination of the Angular Variable

The angular variable is eliminated by projecting the transport equation onto the set of spherical harmonics $\{Y_k^l\}$. Applying the projection operators (5) to integral Eq. (13) yields an infinite set of integral equations

$$\psi_k = T_k(q + S_-) \ , \quad k = 0, 1, \ldots \ , \tag{103}$$

where T_k is the integral operator with kernel $Q_k t$, and

$$\psi_k = Q_k \psi = \sum_{|l| \leq k} \psi_k^l(\mathbf{r}) Y_k^l(\mathbf{\Omega})$$

is the component of the angular flux on the subspace $\mathcal{E}_k$. In terms of these components, the angular

[103]E. E. LEWIS and C. D. SWANSON, "Comparison of Vector Computer Methods for the Solution of Slab Geometry Neutron Transport Problems," *Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems*, Munich, Germany, April 27-29, 1981, Vol. 2, p. 549, Kernforschungszentrum Karlsruhe (1981).

[104]J. R. ASKEW, "Some Boundary Condition Problems Arising in the Application of Collision Probability Methods," *Proc. Sem. Numerical Reactor Calculations*, Vienna, January 17-21, 1972, p. 343, International Atomic Energy Agency (1972).

[105]D. EMENDÖRFER, "Physics Assumptions and Applications of Collision Probability Methods," *Proc. Conf. Mathematical Models and Computational Techniques for Analysis of Nuclear Systems*, Ann Arbor, Michigan, April 9-11, 1973, CONF-730414, p. VIII-136, U.S. Atomic Energy Commission (1974).

[106]A. LEONARD, "Collision Probabilities and Response Matrices: An Overview," *Proc. Conf. Computational Methods in Nuclear Engineering*, Charleston, South Carolina, April 15-17, 1975, CONF-750413, Vol. II, p. III-15, U.S. Energy Research and Development Administration (1975).

[107]T. LEFVERT, *Prog. Nucl. Energy*, **4**, 97 (1979).

[108]A. KAVENOKY, "Status of Integral Transport Theory," *Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems*, Munich, Germany, April 27-29, 1981, Vol. 1, p. 133, Kernforschungszentrum Karlsruhe (1981).

flux can be written as

$$\psi = (4\pi)^{-1}\,[\phi(\boldsymbol{r}) + 3\boldsymbol{\Omega}\cdot\boldsymbol{J}(\boldsymbol{r})] + \sum_{k\geq 2}\psi_k \ ,$$

where only the total flux $\phi(\boldsymbol{r})$ and the net current $\boldsymbol{J}(\boldsymbol{r})$ have direct physical interpretations.

The system of Eqs. (103) is coupled through the angular emission density q. With the aid of Eqs. (4) and (15), q is written as

$$q = \sum_{k=0}^{K}(2k+1)^{-1}\Sigma_{sk}\psi_k + S \ ,$$

where K is the degree of scattering anisotropy. Consequently, in contrast to the spherical harmonics formulation, the integral equations naturally separate into two sets: a closed system of $(K+1)^2$ integral equations for the unknown ψ_k^l, $|l| \leq k \leq K$, and an infinite set of equations for $k > K$ giving the remaining components in terms of the ψ_k^l, $k \leq K$. For a convex body, the closed system of integral equations can be written explicitly, using Eq. (17), as

$$\psi_k^l(\boldsymbol{r}) = \int_D \frac{e^{-\tau}}{s^2}\,[Y_k^l(\boldsymbol{\Omega}_s)]^* q(\boldsymbol{r}',\boldsymbol{\Omega}_s)d\boldsymbol{r}'$$

$$+ \int_{4\pi} e^{-\tau_-}\,[Y_k^l(\boldsymbol{\Omega})]^*\psi_-(\boldsymbol{r}_b,\boldsymbol{\Omega})d\boldsymbol{\Omega} \ ,$$

$$0 \leq |l| \leq k \leq K \ . \quad (104)$$

As before, $\boldsymbol{\Omega}_s = \boldsymbol{s}/s$ with $\boldsymbol{s} = \boldsymbol{r} - \boldsymbol{r}'$, and ψ_- is the incident flux at the point $\boldsymbol{r}_b$ on the surface.

Although Eqs. (104) involve only integral operators over space, their solution becomes overwhelmingly complex even for small K. Therefore, we restrict our attention to $K \leq 1$. For linearly anisotropic scattering, the angular emission density becomes

$$q = (4\pi)^{-1}[\Sigma_{s0}\phi(\boldsymbol{r}) + \Sigma_{s1}\boldsymbol{\Omega}\cdot\boldsymbol{J}(\boldsymbol{r})] + S \ . \quad (105)$$

Hence the closed system of Eqs. (104) reduces to

$$\phi = 4\pi Gq + \phi_0$$

and

$$\boldsymbol{J} = 4\pi G(\boldsymbol{\Omega}q) + \boldsymbol{J}_0 \ . \quad (106)$$

In these equations, G is the integral operator

$$(Gf)(\boldsymbol{r}) = \int g(\boldsymbol{r}'\to\boldsymbol{r})f(\boldsymbol{r}',\boldsymbol{\Omega}_s)d\boldsymbol{r}'$$

defined in terms of the symmetric kernel

$$g(\boldsymbol{r}'\to\boldsymbol{r}) = \frac{e^{-\tau}}{4\pi s^2} \ . \quad (107)$$

The uncollided flux ϕ_0 and net current $\boldsymbol{J}_0$ due to the neutrons entering from the boundaries are

$$\phi_0 = \int e^{-\tau_-}\,\psi_-(\boldsymbol{r}_b,\boldsymbol{\Omega})d\boldsymbol{\Omega}$$

and

$$\boldsymbol{J}_0 = \int \boldsymbol{\Omega}e^{-\tau_-}\psi_-(\boldsymbol{r}_b,\boldsymbol{\Omega})d\boldsymbol{\Omega} \ . \quad (108)$$

As can be seen by these equations, an inherent advantage of the integral transport approach is that the flux and net current can be directly obtained without a detailed calculation of the angular flux, as opposed to the integrodifferential transport formulation.

III.B. General Solution Methods

In this section, the DIT, the collocation, and the CP methods are examined for the case of isotropic scattering and sources. Furthermore, to simplify the discussion, the boundary contribution ϕ_0 is neglected for the moment. Then the transport equation with isotropic scattering and sources becomes the so-called Peierls equation

$$\phi = GF \ , \quad (109)$$

where the volumetric emission density $F(\boldsymbol{r})$,

$$F = \Sigma_{s0}\phi + S_t \ ,$$

includes the contribution from the total volumetric source, which is now $S_t = 4\pi S$.

III.B.1. Three Numerical Approximations

A straightforward attack on integral Eq. (109) follows by using the numerical quadrature technique discussed in Sec. I.C. This procedure leads to the DIT method.[109,110] With the quadrature set $\{\boldsymbol{r}_i, V_i,\ i = 1 \text{ to } N\}$, we obtain a system of algebraic equations for the values of the flux at the nodes $\boldsymbol{r}_i$,

$$\phi_i = \sum_j P_{ij}V_jF_j \ , \quad i = 1 \text{ to } N \ . \quad (110)$$

Here the index i denotes the value of ϕ and F at the i'th node, and

$$P_{ij} = g(\boldsymbol{r}_j\to\boldsymbol{r}_i) \ , \quad j \neq i \ , \quad (111)$$

is the uncollided flux at point $\boldsymbol{r}_i$ created by a unit isotropic source at point $\boldsymbol{r}_j$. Since $g(\boldsymbol{r}\to\boldsymbol{r})$ in Eq. (107) is singular, P_{ii} cannot be calculated with Eq. (111). One approach for removing the singularity is to use the method of Eq. (31); the previous equations remain valid and[111,112]

$$P_{ii} = V_i^{-1}\left[(G1)(\boldsymbol{r}_i) - \sum_{j\neq i}V_jP_{ij}\right] \ . \quad (112)$$

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[109] I. CARLVIK, *Nukleonik*, **10**, 104 (1967).

[110] K. KOBAYASHI and H. NISHIHARA, *J. Nucl. Energy*, **18**, 513 (1964).

The precision of the numerical integration is affected by the irregularities of $g(\mathbf{r}' \to \mathbf{r})F(\mathbf{r}')$. For bodies comprised of homogeneous regions, F is continuous except at interfaces between regions, which suggests that (in one-dimensional geometries) a separate Gauss quadrature formula be applied to each region.

Let us now consider the use of the collocation and projection techniques for the treatment of the Peierls equation. The first step is to select the representation functions $\{f_i,\ i = 1 \text{ to } N\}$ used in the expansion for the flux

$$\phi = \sum_i \phi_i f_i \ . \tag{113}$$

To ensure a good approximation, representation functions with homogeneous support are chosen: The body is subdivided into homogeneous zones and ϕ is approximated by a finite expansion on each zone.

The simplest approximation, in which only one function is used on every zone, is the flat-flux approximation. For this approximation we take

$$f_i(\mathbf{r}) = \begin{cases} 1 \ , & r \in D_i \ , \\ 0 \ , & \text{otherwise} \ , \end{cases} \tag{114}$$

where D_i is the domain of the i'th zone; then the ϕ_i can be interpreted as the average flux in zone i. If we select only one point $\mathbf{r}_i$ per zone, the collocation method gives a system of equations similar to that in Eq. (110) provided we interpret the P_{ij} as

$$P_{ij} = V_j^{-1} \int g(\mathbf{r}' \to \mathbf{r}_i) f_j(\mathbf{r}') d\mathbf{r}' \ , \tag{115}$$

where V_j is the volume of the j'th zone. That is, P_{ij} is the uncollided flux at $\mathbf{r}_i$ created by a unit isotropic source uniformly distributed in zone j (Refs. 113 and 114).

The projection method also yields Eq. (110), but now

$$P_{ij} = (V_i V_j)^{-1} \int f_i(\mathbf{r}) d\mathbf{r} \int g(\mathbf{r}' \to \mathbf{r}) f_j(\mathbf{r}') d\mathbf{r}' \ . \tag{116}$$

The physical interpretation of this P_{ij} follows by considering the product $\Sigma_i P_{ij}$, where Σ_i is the total macroscopic cross section in zone i. This product is the first-flight collision probability in zone i for neutrons uniformly and isotropically emitted from zone j. For this reason, the method is known as the CP method.[115-119]

III.B.2. Incorporation of Boundary Conditions

The previous results can be extended in a direct manner to include the effects of two boundary conditions. First we consider the use of the white boundary condition defined in Eq. (12). This condition is a homogeneous boundary condition and therefore, as shown in Eq. (19), it can be included in the definition of the integral operator. With the aid of the reflected kernel of Eq. (20), we again derive Peierls equation for isotropic scattering and sources, but the kernel of the new operator $\bar{G}$ is

$$\bar{g}(\mathbf{r}' \to \mathbf{r}) = g(\mathbf{r}' \to \mathbf{r}) + \frac{\beta}{1 - \beta P_{SS}} P(\mathbf{r}' \to S) P(S \to \mathbf{r}) \ .$$

In this equation, with the notation of Eq. (20),

$$P(\mathbf{r} \to S) = (A/4)P(S \to \mathbf{r}) = (4\pi)^{-1} \int \exp[-\tau_+(x)] d\boldsymbol{\Omega} \ ,$$

where we recall that A is the surface area of the body. Physically $P(\mathbf{r} \to S)$ is the first-flight escape probability for neutrons isotropically emitted at $\mathbf{r}$, and $P(S \to \mathbf{r})$ is the total uncollided flux at $\mathbf{r}$ produced by one neutron entering the body uniformly and isotropically.

The three approximation methods can be applied to the modified Peierls equation to again obtain the system of Eqs. (110), but with new matrix coefficients

$$\bar{P}_{ij} = P_{ij} + \frac{\beta}{1 - \beta P_{SS}} P_{Sj} P_{iS} \ , \tag{117}$$

where P_{SS} is the transmission probability in Eq. (21). In this equation, for the DIT method, we have

$$P_{Si} = (A/4)P_{iS} = P(\mathbf{r}_i \to S) \ , \tag{118}$$

whereas for the CP method

$$P_{Si} = (A/4)P_{iS} = V_i^{-1} \int P(\mathbf{r} \to S) f_i(\mathbf{r}) d\mathbf{r} \ . \tag{119}$$

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[111]S. K. LOYALKA, *Nucl. Sci. Eng.*, **56**, 317 (1975).

[112]S. K. LOYALKA and R. W. TSAI, *Nucl. Sci. Eng.*, **58**, 193 (1975).

[113]E. E. LEWIS, *J. Nucl. Energy*, **23**, 87 (1969).

[114]T. BOŠEVSKI, *Nucl. Sci. Eng.*, **42**, 23 (1970).

[115]H. HONECK, "THERMOS: A Thermalization Transport Theory Code for Reactor Lattice Calculations," BNL-5826, Brookhaven National Laboratory (1961); see also *Nucl. Sci. Eng.*, **8**, 193 (1960).

[116]R. BONALUMI, *Energ. Nucl.*, **8**, 326 (1961).

[117]Y. FUKAI, *React. Sci. Technol.*, **17**, 115 (1963).

[118]I. CARLVIK, "A Method for Calculating Collision Probabilities in General Cylindrical Geometry and Applications to Flux Distributions and Dancoff Factors," *Proc. Third Int. Conf. Peaceful Uses of Atomic Energy*, Geneva, Switzerland, August 31–September 9, 1964, Vol. 2, p. 225, United Nations, New York (1965).

[119]A. KAVENOKY, "Calcul et Utilisation des Probabilités de Première Collision pour des Milieux Hétérogènes à Une Dimension," CEA N-1077, Commissariat à l'Energie Atomique (1969).

The quantities in the last equation have a direct physical meaning. The P_{Si} is the first-flight escape probability for neutrons uniformly and isotropically born in zone i, and $\Sigma_i P_{iS}$ is the probability that neutrons entering the body uniformly and isotropically will suffer their first collision in zone i. For the collocation method, P_{Sj} in Eq. (117) has the form given in Eq. (118), while P_{iS} is the one defined in Eq. (119).

The second boundary condition we consider is that of a body uniformly and isotropically irradiated with a constant angular flux ψ_0. This is an inhomogeneous boundary condition, and hence we have to include the surface contribution in the Peierls equation

$$\phi = GF + \phi_0 \ .$$

With the aid of Eq. (108), the inhomogeneous term may be written in terms of the total incident current $\pi A \psi_0$ as

$$\phi_0 = \pi A \psi_0 P(S \to \boldsymbol{r}) \ .$$

Again all three numerical methods give a set of equations analogous to Eq. (110),

$$\phi_i = \sum_j P_{ij} V_j F_j + \pi A \psi_0 P_{iS} \ , \quad i = 1 \text{ to } N \ . \tag{120}$$

III.B.3. Reciprocity and Conservation Relations

General properties of the solutions of the linear transport equation should be employed to reduce the amount of work needed to calculate the P_{ij}, P_{Si}, P_{iS}, and P_{SS}. Although reciprocity relations are usually derived from the reciprocity of the Green's function,[4] for the transport of uncollided neutrons they result simply from the symmetry of the optical distance $\tau(\boldsymbol{r},\boldsymbol{r}') = \tau(\boldsymbol{r}',\boldsymbol{r})$. In the DIT and CP methods, reciprocity leads to the symmetry relation

$$P_{ij} = P_{ji} \ , \tag{121}$$

which is also valid for the "reflected" probabilities $\bar{P}_{ij}$ in Eq. (117), so that only the P_{ij} (or $\bar{P}_{ij}$), $i \leqslant j$, need to be calculated. For these two methods, the symmetry between P_{Si} and P_{iS} shown in Eqs. (118) and (119) is also due to reciprocity.

Conservation principles are formally obtained by weighted integration of the Green's function Eq. (14), but for uncollided neutrons one can take advantage of the fact that the medium appears to be purely absorbing. In this latter case, the emission term $H\psi$ in the integrodifferential Eq. (1) can be suppressed and integration over the entire phase space gives

$$\int_{\partial D} \boldsymbol{J}_u \cdot d\boldsymbol{A} = \int_D (S_t - \Sigma \phi_u) d\boldsymbol{r} \ , \tag{122}$$

where $\boldsymbol{J}_u(\boldsymbol{r})$ and $\phi_u(\boldsymbol{r})$ are the uncollided net current and flux resulting from the angular source $S(\boldsymbol{r},\boldsymbol{\Omega})$ of total intensity $S_t(\boldsymbol{r})$.

We first apply this equation to the DIT method. With $S(\boldsymbol{r},\boldsymbol{\Omega}) = (4\pi)^{-1}\delta(\boldsymbol{r} - \boldsymbol{r}_j)$ and using the numerical quadrature for the integral of $\Sigma\phi_u$, we obtain

$$P_{Sj} = 1 - \sum_i \Sigma_i V_i P_{ij} \ . \tag{123}$$

Similarly, in the CP method, the same equation is obtained (without the numerical integration) with the source $S(\boldsymbol{r},\boldsymbol{\Omega}) = (4\pi V_j)^{-1} f_j(\boldsymbol{r})$. Furthermore, with an incoming surface source given by $S(\boldsymbol{r},\boldsymbol{\Omega}) = -(\pi A)^{-1}(\boldsymbol{\Omega}\cdot\boldsymbol{n})\delta_-(x)$, Eq. (122) yields

$$P_{SS} = 1 - \sum_i \Sigma_i V_i P_{iS} \ , \tag{124}$$

for both methods (where again the numerical integration has been used for the DIT formulation).

In the DIT method, Eq. (123) provides an alternative to Eq. (112) for the calculation of the diagonal elements P_{ii} in terms of the P_{ij}, $i \neq j$, and P_{Si} which can be directly computed. Indeed, such a technique was used by Carlvik in the original DIT method[109] and provides better results, at least for plane geometry, than those from the use of Eq. (112).

III.B.4. Comparisons

The three numerical solution methods may be compared from three points of view: their ability to provide a good approximation for the flux, the numerical effort required to calculate the elements P_{ij} of the collision matrix, and the treatment of boundary conditions.

The collocation and CP methods are based on a direct approximation of the flux, as in Eq. (113). On the other hand, the approximation underlying the DIT method is equivalent to a piecewise polynomial interpolation of the product $g(\boldsymbol{r}' \to \boldsymbol{r})\phi(\boldsymbol{r}')$, which tends to be less regular than the flux.

For the DIT method, the calculation of P_{ij} requires only the evaluation of an exponential function, whereas one integration is required in the collocation approach and two are needed in the CP method. In the DIT and CP methods, the reciprocity relation reduces by nearly a factor of 2 the number of P_{ij} to be calculated, so only $N(N+1)/2$ coefficients have to be computed instead of the N^2 required for the collocation method.

For boundary conditions involving uniform and isotropic angular distributions, conservation relations (123) and (124) and the reciprocity between P_{Sj} and P_{jS} can be used to obtain the matrix coefficients P_{Sj}, P_{jS}, and P_{SS} for the DIT and CP methods. Moreover, for a perfectly reflecting surface ($\beta = 1$), these relations ensure neutron conservation, a fact that is crucial for cell calculations. For the collocation method, however, each matrix coefficient must be individually calculated; furthermore, to guarantee

neutron conservation, the conservation equations must be used to normalize the set of coefficients.

Although the implementation of the CP method is more complicated, this method is by far the most used of the three. For this reason, we will focus on this scheme from now on.

III.C. Collision Probability Method

Even with isotropic scattering and sources, the solution of the integral equation for a general geometry is a formidable task. If the geometry, sources, and boundary conditions have the appropriate symmetries, however, the transport equation can be simplified. This is the case for the three one-dimensional geometries (plane, cylindrical, and spherical) and the Cartesian x-y geometry, which we consider in this section.

In one-dimensional geometries, the cross sections depend on only one principal (spatial) coordinate ξ and the transport equation can be reduced to an integral equation involving only ξ. The principal coordinate ξ is given in Table II for the three geometries: plane ($\alpha = 0$), cylindrical ($\alpha = 1$), and spherical ($\alpha = 2$). For the case of isotropic scattering and sources, the Peierls equation can be written as

$$\phi = G_\alpha F \ , \tag{125}$$

where ϕ and F depend only on ξ. The integral operator G_α is defined as[22]

$$G_\alpha f = \int_{D_\xi} g_\alpha(\xi' \to \xi) f(\xi')(\xi')^\alpha d\xi' \ , \tag{126}$$

where the domain D_ξ is in Table II. The kernel g_α is obtained from the kernel g of the general integral operator as

$$g_\alpha(\xi' \to \xi) = (\xi')^{-\alpha} \int_{S_{\xi'}} g(\boldsymbol{r}' \to \boldsymbol{r}) dA' \ .$$

In this expression the integration is performed over the surface $S_{\xi'}$ containing all points with principal coordinate ξ'.

Physically, the kernel $g_\alpha(\xi' \to \xi)$ is the uncollided flux at a point $\boldsymbol{r}$ with principal coordinate ξ produced by an isotropic source uniformly distributed over the surface $S_{\xi'}$ which emits $(\xi')^{-\alpha}$ n/cm^2. In the three geometries, the kernels g_α are[119,120]

$$g_\alpha(\xi' \to \xi) = \begin{cases} \frac{1}{2} E_1(|\tilde{\xi} - \tilde{\xi}'|) \ , & \alpha = 0 \\ \frac{1}{\pi} \int_0^{\xi<} \frac{dR}{tt'} \left[Ki_1(\tilde{t} + \tilde{t}') + Ki_1(|\tilde{t} - \tilde{t}'|) \right] \ , & \alpha = 1 \\ \frac{1}{2\pi\xi\xi'} \int_0^{\xi<} \frac{RdR}{tt'} \{ \exp[-(\tilde{t} + \tilde{t}')] + \exp(-|\tilde{t} - \tilde{t}'|) \} \ , & \alpha = 2 \ . \end{cases} \tag{127}$$

In plane geometry, the kernel depends on the exponential integral function,[1]

$$E_n(x) = \int_0^1 \exp(-x/t) t^{n-2} dt \ ,$$

and $\tilde{\xi}$ is the optical distance in direction z between the plane of principal coordinate $z = \xi$ and an arbitrary reference plane. In cylindrical geometry, the kernel requires calculation of the Bickley-Naylor function[121]

$$Ki_n(x) = \int_0^{\pi/2} \exp(-x/\sin\theta)(\sin\theta)^{n-1} d\theta \ .$$

For both cylindrical and spherical geometries, $\xi< = \min(\xi, \xi')$, $t = (\xi^2 - R^2)^{1/2}$ is the distance OP in Fig. 1, and $\tilde{t}$ is the corresponding optical distance.

We now consider the application of the CP method for multilayered one-dimensional geometries. Then we may order the zones in increasing values of the principal coordinate so that the i'th zone corresponds to $\xi_i \leqslant \xi \leqslant \xi_{i+1}$, with $\xi_1 = -a$ in plane geometry and 0 otherwise, and $\xi_{N+1} = a$. For the flat-flux approximation of Eq. (114), the fluxes ϕ_i satisfy the system of Eqs. (110). After eliminating superfluous integrations over infinite domains, the collision probabilities of Eq. (116) become

$$P_{ij} = \omega(V_i V_j)^{-1} \int_{\xi_i}^{\xi_{i+1}} \xi^\alpha d\xi \int_{\xi_j}^{\xi_{j+1}} g_\alpha(\xi' \to \xi)(\xi')^\alpha d\xi' \ . \tag{128}$$

Here the "volumes" are

$$V_i = \omega \int_{\xi_i}^{\xi_{i+1}} (\xi')^\alpha d\xi' = \frac{\omega}{\alpha + 1} (\xi_{i+1}^{\alpha+1} - \xi_i^{\alpha+1}) \ , \tag{129}$$

and the ω values are given in Table II.

TABLE II

Notation for One-Dimensional Geometries

Geometry	α	Principal Coordinate ξ	Domain D_ξ	ω
Plane	0	Depth z	$[-a,a]$	1
Cylindrical	1	Radius ρ	$[0,a]$	2π
Spherical	2	Radius r	$[0,a]$	4π

[120]R. SANCHEZ, "Application de la Méthode de Galerkin à la Résolution de l'Equation Intégrale du Transport Unidimensionnelle," CEA-N-1793, Commissariat à l'Energie Atomique (1974).

[121]W. G. BICKLEY and J. NAYLOR, *Philos. Mag.*, **20**, 343 (1935).

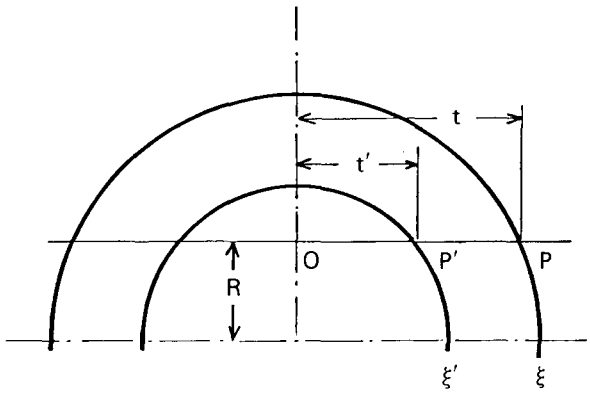

Fig. 1. Explanation of symbols for $g_\alpha(\xi' \to \xi)$ in cylindrical and spherical geometries. In cylindrical geometry the figure represents a cross section normal to the axis of symmetry; in spherical geometry it represents a cross section passing through the origin. (The length t is the distance OP and $\tilde{t}$ is the optical distance OP.)

The main task in the implementation of the CP method lies in the calculation of the collision probabilities, which we now discuss for the three one-dimensional geometries.

III.C.1. Plane Geometry

In this geometry, the argument of the exponential integral function is linear in ξ and ξ':

$$\tilde{\xi} - \tilde{\xi}' = \tilde{\xi}_i - \tilde{\xi}_j + \Sigma_i(\xi - \xi_i) - \Sigma_j(\xi' - \xi_j) \ . \quad (130)$$

Then, using the formula $dE_{n+1}(x)/dx = -E_n(x)$, the two integrations in Eq. (128) can be done analytically. Each of the integrations increases by one the order of the exponential integral function. The resulting flat-flux collision probabilities are written, in concise notation, as

$$P_{ij} = \begin{cases} (\Sigma_i V_i)^{-1}[-(2\Sigma_j V_j)^{-1} H_{ij} E_3(|\tilde{\xi} - \tilde{\xi}'|) + \delta_{ij}] \ , \\ \qquad \Sigma_i, \Sigma_j \neq 0 \\ (2\Sigma_i V_i)^{-1} \operatorname{sgn} H_i E_2(|\tilde{\xi} - \tilde{\xi}_j|) \ , \\ \qquad \Sigma_i \neq 0 \ , \quad \Sigma_j = 0 \ . \end{cases} \quad (131)$$

Here, sgn is the sign of $(\xi_j - \xi_i)$, H_i and its counterpart H_j' are the difference operators

$$H_i f(\xi, \xi') = f(\xi_{i+1}, \xi') - f(\xi_i, \xi')$$

and

$$H_j' f(\xi, \xi') = f(\xi, \xi_{j+1}) - f(\xi, \xi_j) \ , \quad (132)$$

and H_{ij} acts as the operator $H_i H_j'$ and therefore gives rise to four terms.

Although in general each P_{ij} requires the calculation of four exponential integral functions, the total number of functions to be evaluated is nearly halved by virtue of the common terms. In practice, values of a given exponential integral function can be directly calculated using a rational or polynomial expansion or, if there is sufficient computer memory, by interpolation from tabulated values. Once the E_3 values are known, the E_2 values can be calculated, if needed, from the recursion relation

$$E_{n+1}(x) = [e^{-x} - xE_n(x)]/n \ , \quad n \geq 1 \ . \quad (133)$$

In lattice calculations, specular reflection at the surfaces of the cell is handled by extending the domain of integration to infinity by repeated symmetries of the original cell. Then, for a given zone i, the collision probability P_{ij} is calculated by integration over zone j and all its images until the next layer makes a negligible contribution.[6] Less physical boundary conditions that involve isotropic incident angular distributions can be treated in the manner discussed in Sec. III.B.

III.C.2. Cylindrical and Spherical Geometries

For these geometries, since the kernel is defined in terms of an integral, the collision probabilities in Eq. (128) involve three integrations. The order of integration is interchanged so that the integrals over ξ and ξ' can be done first. Then, changing variables to t and t', respectively, and observing that $(\tilde{t} \pm \tilde{t}')$ is linear in t and t' [in a manner similar to Eq. (130)], the integrations in t and t' can be performed analytically. The result is

$$P_{ij} = (\Sigma_i V_i)^{-1} \left[\int_0^{r<} F_{ij}(R) R^{\alpha-1} dR + \delta_{ij} \right] \ , \quad (134)$$

where $r< = \min(\xi_{i+1}, \xi_{j+1})$.

In cylindrical geometry, the $F_{ij}(R)$ are

$$F_{ij} = \begin{cases} -2(\Sigma_j V_j)^{-1} H_{ij}[Ki_3(|\tilde{t} - \tilde{t}'|) - Ki_3(\tilde{t} + \tilde{t}')] \ , \\ \qquad \Sigma_i, \Sigma_j \neq 0 \ , \\ 2V_j^{-1}(t_{j+1} - t_j) H_i[\operatorname{sgn} Ki_2(|\tilde{t} - \tilde{t}'|) \\ \quad - Ki_2(\tilde{t} + \tilde{t}')] \ , \quad \Sigma_i \neq 0 \ , \quad \Sigma_j = 0 \ , \end{cases}$$

where the notation is that of Eq. (132) and Fig. 1, and use has been made of the formula $dKi_{n+1}/dx = -Ki_n(x)$. The corresponding expressions in spherical geometry are

$$F_{ij} = \begin{cases} -2\pi(\Sigma_j V_j)^{-1} H_{ij}\{\exp(-|\tilde{t} - \tilde{t}'|) - \exp[-(\tilde{t} + \tilde{t}')]\} \ , \\ \qquad \Sigma_i, \Sigma_j \neq 0 \\ 2\pi V_j^{-1}(t_{j+1} - t_j) H_i\{\operatorname{sgn} \exp(-|\tilde{t} - \tilde{t}'|) \\ \quad - \exp[-(\tilde{t} + \tilde{t}')]\} \ , \quad \Sigma_i \neq 0 \ , \quad \Sigma_j = 0 \ . \end{cases}$$

The integration over R in Eq. (134) must be done numerically, but some precautions must be taken to avoid a loss of precision caused by a singular behavior of the integrand. For example, in the calculation of P_{ii} and $P_{i,i+1}$, the argument $(\tilde{t}_{i+1} - \tilde{t}_i)$ vanishes as R

approaches the upper limit of integration ξ_{i+1} and this causes the integrand to have an unbounded derivative at that point. To avoid the loss of precision, the integral is decomposed such that

$$\int_0^{\xi_{i+1}} f(R)dR = \sum_{k=1}^{i} \int_{\xi_k}^{\xi_{k+1}} f(R)dR \ .$$

Then, after elimination of the singularity by a change of variables with $R = \xi_{k+1} - x^2$, each integral on x is done with a Gauss-Legendre formula.[118]

For every integration node, each P_{ij} requires calculation of up to eight functions, but again this number can be reduced by nearly a factor of 2 by careful numerical programming. For cylindrical geometry, the calculation of the Ki functions can be performed using either rational[122] or polynomial expansions, or tabulated values. It should be mentioned that for a homogeneous sphere the integration over R in Eq. (134) can be done analytically in terms of the exponential integral functions of order 3, 4, and 5.

Let us now consider the treatment of boundary conditions. For white boundary conditions, the most expedient approach is to replace the collision probabilities by those of Eq. (117). Then all the surface coefficients P_{SS}, P_{Sj}, and P_{iS} can be evaluated using reciprocity relation (119) and the conservation equations (123) and (124). In the case of an inhomogeneous, isotropic-boundary condition, the same procedure will yield the P_{iS} in the surface terms of Eq. (120).

III.C.3. Two-Dimensional Cartesian Geometry

Another case in which the integral equation can be reduced to a manageable form is that of a geometry in which the cross sections, sources, and boundary conditions are independent of z. Also, often the sources and boundary conditions (and thus the angular flux) are taken to be symmetric in angle with respect to the xy plane. Then, for isotropic scattering and sources, Peierls' Eq. (109) appears as

$$\phi = G_{xy}F \ , \qquad (135)$$

where the emission density and flux depend on the two-dimensional variable $\boldsymbol{\xi} = (x,y)$. The integral operator G_{xy} is

$$G_{xy}f = \int g_{xy}(\boldsymbol{\xi}' \to \boldsymbol{\xi}) f(\boldsymbol{\xi}')d\boldsymbol{\xi}' \ ,$$

with kernel

$$g_{xy}(\boldsymbol{\xi}' \to \boldsymbol{\xi}) = \int_{-\infty}^{\infty} g(\boldsymbol{r}' \to \boldsymbol{r})dz' = \frac{Ki_1(\tau_{xy})}{2\pi|\boldsymbol{\xi}' - \boldsymbol{\xi}|} \ .$$

[122] I. GARGANTINI and T. POMENTALE, *Comm. Assoc. Computing Mech.*, **7**, 727 (1964).

Here τ_{xy} is the optical distance measured in the xy plane between $\boldsymbol{\xi}'$ and $\boldsymbol{\xi}$, the projections of $\boldsymbol{r}'$ and $\boldsymbol{r}$. Physically, g_{xy} represents the uncollided flux at $\boldsymbol{r}$ due to an isotropic line source, of unit magnitude per unit length, which passes in the z direction through the point $\boldsymbol{\xi}'$.

To apply the CP method to this geometry, the two-dimensional domain of the $\boldsymbol{\xi}$ variable is decomposed into homogeneous zones. As before, the use of the flat-flux approximation gives the system of Eqs. (110) with

$$P_{ij} = (V_i V_j)^{-1} \int_{D_i} d\boldsymbol{\xi} \int_{D_j} g_{xy}(\boldsymbol{\xi}' \to \boldsymbol{\xi})d\boldsymbol{\xi}' \ ,$$

where D_i is the domain of the i'th zone of volume V_i. The analytical evaluation of this expression is simplified when the integration is performed following the projection of the neutron trajectories on the xy plane (i.e., from $\boldsymbol{\xi}'$ to $\boldsymbol{\xi}$). To do so, the coordinates are changed from $(\boldsymbol{\xi}', \boldsymbol{\xi})$ to (R,ϕ,t,t') as shown in Fig. 2. The Jacobian of this transformation is $|\boldsymbol{\xi}' - \boldsymbol{\xi}|/\xi\xi'$, so that

$$P_{ij} = (2\pi V_i V_j)^{-1} \int Ki_1(\tau_{xy})dRd\phi dtdt' \ . \qquad (136)$$

Along the line of integration defined by fixed R and ϕ, the optical distance τ_{xy} is linear in t' and t. Hence, the integration over these two variables can be done analytically to yield

$$P_{ij} = (\Sigma_i V_i)^{-1} \left[\int F_{ij}(R,\phi)dRd\phi + \delta_{ij} \right] \ , \qquad (137)$$

where

$$F_{ij}(R,\phi) = \begin{cases} -(2\pi\Sigma_j V_j)^{-1} H_{ij} Ki_3(|\tilde{t} - \tilde{t}'|) \ , \\ \qquad\qquad \Sigma_i, \Sigma_j \neq 0 \\ (2\pi V_j)^{-1}(t_{j+1} - t_j) H_i \ \mathrm{sgn} \ Ki_2(|\tilde{t} - \tilde{t}'|) \ , \\ \qquad\qquad \Sigma_i \neq 0 \ , \quad \Sigma_j = 0 \ . \end{cases}$$

Here, $\tilde{t}$ is the optical distance along the line of integration corresponding to t, and t_i and t_{i+1} are the coordinates of the intersection of this line with the boundary of zone i (see Fig. 2).

A special case arises if the geometry is invariant under rotation, so that the zones i and j can be chosen to be annuli. Then the ϕ integration yields a factor of 2π and Eq. (137) reduces to the one-dimensional cylindrical geometry form obtained before. The integrations in Eq. (137) must be carried out numerically. To minimize the number of Ki functions to be evaluated, a single mesh of integration is used for all the P_{ij}. In practice, the trapezoidal integration formula with equal weights is used for both R and ϕ to define the mesh of integration. Implementation of this integration scheme requires

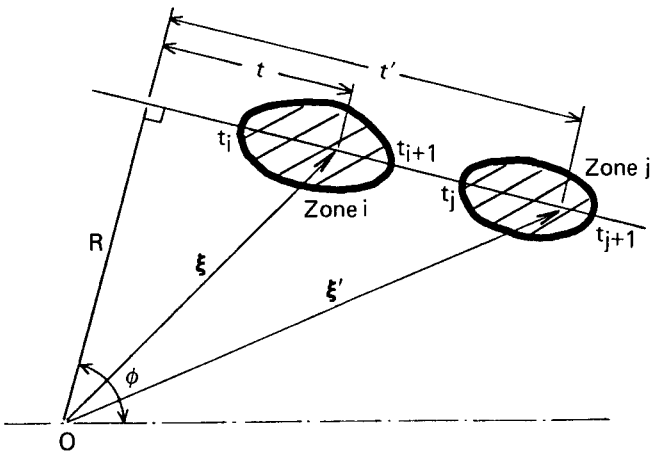

Fig. 2. Schematic diagram of natural coordinates for two-dimensional geometry.

development of a computer "tracking" subroutine for calculating the intersection of the lines of integration with all the zones. To maximize computing efficiency, specialized subroutines are developed for each different geometrical configuration.[123-128] Nevertheless, this geometric calculation can be quite time consuming and, in a multigroup problem, the computation of the P_{ij} is done in two stages: First, the tracking subroutine is used and the geometric data are stored, and then these data, together with the cross sections, are used to calculate the P_{ij} for every energy group.

Finally, it should be mentioned that the CP method also has been used for the treatment of a two-dimensional r-z geometry.[129,130]

III.C.4. Multifunction Expansions

The flat-flux CP approximation converges toward the exact solution as the number of zones N increases. Since the number of P_{ij} to be computed varies as N^2, the calculation of an optically large medium, or one in which there is a strong flux gradient, can become impractical. This problem is further aggravated if a numerical integration is needed in the calculation of the P_{ij}; for instance, in cylindrical geometry, the number of Bickley-Naylor functions to be evaluated varies as N^3. To improve the efficiency of the CP method in such cases, two variations have been developed. One approach is to use more than one expansion function per zone, so that local flux gradients can be taken into account; a second approach is to subdivide the optically large media into subdomains or cells that can be efficiently treated with the CP method, and couple the solutions via interface currents as discussed in Sec. III.F.

The rate of convergence of the CP method can be improved if more than one expansion function is used per zone to construct an approximation for the flux of the form

$$\phi = \sum_{i,k} \phi_i^k f_i^k \ . \tag{138}$$

As in the flat-flux approximation, the body has been divided into N homogeneous zones denoted by subscript i. The function f_i^k is defined in zone i and vanishes everywhere else, and superscript k, $k = 1$ to K_i, is used to distinguish different functions in the same zone. For convenience, the expansion functions are orthogonalized according to

$$\int f_i^k f_j^l d\boldsymbol{r} = \delta_{ij}\delta_{kl} V_i \ , \tag{139}$$

where V_i is the volume of zone i; to be consistent with the flat-flux approximation, we set $f_i^1 = 1$ in zone i. With expansion (138), the projection technique yields the following system of CP equations for the coefficient ϕ_i^k:

$$\phi_i^k = \sum_{j,l} P_{ij}^{kl} V_j F_j^l \ , \quad i = 1 \text{ to } N \ , \quad k = 1 \text{ to } K_i \ . \tag{140}$$

Here $F_j^l = \Sigma_{s0,j}\phi_j^l + S_{tj}^l$, and the generalized collision probabilities P_{ij}^{kl} are defined as

$$P_{ij}^{kl} = (V_i V_j)^{-1} \int f_i^k(\boldsymbol{r}) d\boldsymbol{r} \int g(\boldsymbol{r}' \to \boldsymbol{r}) f_j^l(\boldsymbol{r}') d\boldsymbol{r}' \ , \tag{141}$$

and satisfy the reciprocity relation $P_{ij}^{kl} = P_{ji}^{lk}$.

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[123]A. AHLIN, "Instructions for the Use of the CLUCOP Programme," RFN-202, ENEA Computer Programme Library (Nov. 1965).

[124]L. AMYOT and P. BENOIST, *Nucl. Sci. Eng.*, **28**, 215 (1967).

[125]K. TSUCHIHASHI, "CLUP 77: A Fortran Program of Collision Probabilities for Square Clustered Assembly," JAERI 1196, Japan Atomic Energy Research Institute (Jan. 1971).

[126]A. J. JANSSEN and L. M. CASPERS, *Atomkernenergie*, **21**, 27 (1973).

[127]D. W. ANDERSON, "The WIMS'E' Module W-PIJ–A Two-Dimensional Collision Probability Code with General Boundary Conditions," AEEW-R 862, U.K. Atomic Energy Authority, Winfrith (1973).

[128]Z. STANKOVSKI, "Dvodimenzion alno Tretiranje Transporta Neutrona u Heterogenoj Sredini Galerkin-Ovom Metodom," Univerzitet u Beogradu, Thesis (Dec. 1977) (in Serbo-Croatian).

[129]H. H. W. PITCHER, "PRIZE: A Program for Calculating Collision Probabilities in *R-Z* Geometry," AEEW-M469, U.K. Atomic Energy Authority, Winfrith (1964).

[130]P. W. JOHNSON and D. L. NUNN, "A New Version of the PRICE Program for Collision Probability Calculations in *R-Z* Geometry," RD/B/N 1410 RPLC/P256, Central Electricity Generating Board (Oct. 1969).

The functions f_i^k must be chosen to provide a reasonable expansion for the flux and, if possible, be such that some of the integrals in Eq. (141) can be performed analytically. In particular, for the three one-dimensional geometries with principal coordinate ξ, these "integrability conditions" require that $f_i^k(\xi)$ be a polynomial in ξ^s of degree k, with $s = 1$ in plane geometry and $s = 2$ in the other two geometries.[22]

For pragmatic reasons, a constant number of expansion functions per zone K_i is used for all zones. This value of K_i should be small, or otherwise there is loss of accuracy in the P_{ij}^{kl}. This is caused by numerical difference effects (i.e., errors arising from taking the numerical difference of two nearly equal numbers). In the past, two terms have been used in the treatment of one-dimensional[120,131,132] and two-dimensional[128] x-y geometries. Even for two-term expansions, one must use double precision to mitigate the numerical difference effects. In plane and cylindrical geometries, multifunction expansions require the evaluation of exponential integral and Bickley-Naylor functions of several orders, respectively; then Eq. (133) and recursion relation

$$(n-1)Ki_n(x) = (n-2)Ki_{n-2}(x) + x\,[Ki_{n-3}(x) - Ki_{n-1}(x)]$$

should be used. It should be mentioned that three-term expansions also have been used with the closely related collocation method.[133,134]

III.D. CP Method with Anisotropic Scattering

In the integral equation formalism, the number of equations to be solved increases rapidly with the degree of anisotropic scattering so a straightforward numerical treatment is impractical. Moderately anisotropic scattering, however, can be approximately included in the formalism by using the so-called "transport correction" to modify the cross sections.[135] Nonetheless, in one-dimensional geometries it is possible to define a "mixed" method,[134] in which some of the integral equations are replaced by differential equations from the P_N formalism. These P_N equations can be analytically integrated to obtain some of the angular moments of the flux and the remaining moments can be calculated by solving integral equations. In particular, in plane geometry, for any degree of scattering anisotropy, all the angular moments may be calculated from the P_N equations in terms of the scalar flux. The flux is then calculated by solving a single integral equation.[22]

A special case considered here is that of the three one-dimensional geometries (for $\alpha = 0$, 1, or 2) with linearly anisotropic scattering and sources. Then, in the notation of Table II, the current is in the direction of the gradient of the principal coordinate ξ, $\boldsymbol{n} = \nabla\xi$, so that a single integral equation for the flux ϕ can be obtained by use of the neutron continuity Eq. (24). Integration over volume of this equation yields

$$J(\xi) = \xi^{-\alpha}\left[J(0) + \int_0^{\xi} C(\xi')(\xi')^{\alpha}d\xi'\right] , \qquad (142)$$

where $C(\xi)$ is the effective volume source $S_t - \Sigma_a\phi$. Here $J(0) = 0$ except for the nonsymmetric slab, in which case $J(0)$ is calculated by specializing the second of Eq. (106) to the origin.

With the aid of Eq. (142), the angular emission density q in Eq. (105) can be explicitly evaluated in terms of the flux. Replacement of the resulting expression for q in the integral equation for the flux yields

$$\phi = G_\alpha F + \hat{G}_\alpha \hat{F} + \phi_0 , \qquad (143)$$

where

$$\hat{F} = \Sigma_{s1}J + S_1 .$$

Here S_1 is the linearly anisotropic component of the source, as defined in the equation

$$S(\boldsymbol{r},\boldsymbol{\Omega}) = (4\pi)^{-1}[S_t(\boldsymbol{r}) + \boldsymbol{\Omega}\cdot\boldsymbol{n}S_1(\boldsymbol{r})] .$$

The integral operator G_α is the one given in Eq. (126), and $\hat{G}_\alpha$ is similarly defined, but with the anisotropic kernel

$$\hat{g}_\alpha(\xi' \to \xi) = (\xi')^{-\alpha}\int_{S_{\xi'}} g(\boldsymbol{r}' \to \boldsymbol{r})\boldsymbol{\Omega}_s\cdot\boldsymbol{n}'dA' .$$

This kernel is the uncollided flux, at a point of principal coordinate ξ, originating from a surface source of the form

$$S(\xi,\boldsymbol{\Omega}) = (4\pi\xi^{\alpha})^{-1}\delta(\xi - \xi')(\boldsymbol{\Omega}\cdot\boldsymbol{n}) .$$

This source has a zero total intensity but a net current of $\boldsymbol{J}(\xi) = (3\xi^{\alpha})^{-1}\delta(\xi - \xi')\boldsymbol{n}$.

For the three one-dimensional geometries, and with the notation of Eq. (127), the anisotropic kernel $\hat{g}$ is[120]

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[131]A.-M. BRUN and A. KAVENOKY, "Acceleration Technique for the Solution of Boltzmann Integral Equation," *Proc. Conf. New Developments in Reactor Mathematics and Applications*, Idaho Falls, Idaho, March 29-31, 1971, CONF-710302, Vol. II, p. 739, U.S. Atomic Energy Commission (1971).

[132]T. TAKEDA and T. SEKIYA, *J. Nucl. Energy*, **27**, 15 (1973).

[133]J. LIGOU, J. STEPANEK, and P. A. THOMI, "Forme Intégrale de l'Equation du Transport-Applications Polynomiales et Diffusion Anisotrope," *Proc. Sem. Numerical Reactor Calculations*, Vienna, January 17-21, 1972, p. 231, International Atomic Energy Agency (1972).

[134]J. LIGOU, *Nucl. Sci. Eng.*, **50**, 135 (1973).

[135]H. LORAIN, "Modèles Synthétiques de Ralentissement des Neutrons et Méthode C_N—Application à l'Interprétation des Expériences Exponentielles Rapides," Université de Paris Sud, Thése Doctorat d'Etat (1972).

$$\hat{g}_\alpha(\xi' \to \xi) = \begin{cases} -\frac{1}{2}\,\mathrm{sgn}\, E_2(|\tilde{\xi} - \tilde{\xi}'|) \ , & \alpha = 0 \\ -\frac{1}{\pi\xi'} \int_0^{\xi<} \frac{dR}{t} \left[Ki_2(\tilde{\tau} + \tilde{\tau}') \right. \\ \quad \left. + \mathrm{sgn}\, Ki_2(|\tilde{\tau} - \tilde{\tau}'|) \right] \ , & \alpha = 1 \\ -\frac{1}{2\pi\xi\xi'} \int_0^{r<} \frac{RdR}{t} \{\exp[-(\tilde{\tau} + \tilde{\tau}')] \\ \quad + \mathrm{sgn} \exp(-|\tilde{\tau} - \tilde{\tau}'|)\} \ , & \alpha = 2 \ , \end{cases} \quad (144)$$

where sgn stands for the sign of $(\xi' - \xi)$.

With the projection technique, the numerical solution of Eq. (143) is accomplished using the multifunction expansion for the flux, as in Eq. (138), and a similar expansion for the isotropic component S_t of the source. The next step is to obtain an expression for $\hat{F}$. First, expansions for the emission density F and the effective source C are directly obtained from those for ϕ and S_t. The expression for C is then substituted into Eq. (142) to yield the current

$$J(\xi) = (\xi_i/\xi)^\alpha J(\xi_i) + \sum_k C_i^k \hat{f}_i^k(\xi) \quad (145)$$

for the zone $\xi_i \leqslant \xi \leqslant \xi_{i+1}$. Here $C_i^k = S_i^k - \Sigma_{ai}\phi_i^k$, and

$$\hat{f}_i^k = \begin{cases} \xi^{-\alpha} \int_{\xi_i}^{\xi} f_i^k(\xi')(\xi')^\alpha d\xi' \ , & \xi_i \leqslant \xi \leqslant \xi_{i+1} \ , \\ 0 \ , \quad \text{otherwise} \ . \end{cases} \quad (146)$$

With the help of orthogonality Eq. (139) and the volume of Eq. (129), we calculate from Eq. (142) the quantity

$$C_i^0 = \xi_i^\alpha J(\xi_i) = J(0) + \omega^{-1} \sum_{j<i} V_j C_j^1 \ , \quad (147)$$

where ω is the angular factor in Table II; this means that the current in Eq. (145) can be written as

$$J(\xi) = \sum_i \left[C_i^0 \xi^{-\alpha} + \sum_{k=1}^{K_i} C_i^k \hat{f}_i^k \right] .$$

Assuming now a similar expression for the anisotropic portion S_1 of the source, one obtains the expansion for $\hat{F}$,

$$\hat{F} = \sum_i \left[\hat{F}_i^0 \xi^{-\alpha} + \sum_k \hat{F}_i^k \hat{f}_i^k \right] ,$$

with the components $\hat{F}_i^k = \Sigma_{s1,i} C_i^k + S_{1,i}^k$ for $k \geqslant 0$.

At this point we have expansions for ϕ, F, and $\hat{F}$, and we can obtain the CP formulation by projecting Eq. (143) onto the expansion functions f_i^k. The result is

$$\phi_i^k = \sum_j V_j \left[\sum_l (P_{ij}^{kl} F_j^l + \hat{P}_{ij}^{kl} \hat{F}_j^l) + \hat{P}_{ij}^{k0} \hat{F}_j^0 \right] + \phi_{0,i}^k \ ,$$
$$i = 1 \text{ to } N \ , \quad k = 1 \text{ to } K_i \ , \quad (148)$$

where the P_{ij}^{kl} are those of Eq. (141) (for one-dimensional geometry). The anisotropic probabilities are defined as

$$\hat{P}_{ij}^{kl} = \omega(V_i V_j)^{-1} \int_{\xi_i}^{\xi_{i+1}} f_i^k(\xi)\xi^\alpha d\xi \int_{\xi_j}^{\xi_{j+1}} \hat{g}_\alpha(\xi' \to \xi) \times \hat{f}_j^l(\xi')(\xi')^\alpha d\xi' \quad (149)$$

for $l > 0$, and by a similar expression for $l = 0$ except that $\hat{f}_j^l(\xi')$ is replaced by $(\xi')^{-\alpha}$.

Next we consider the numerical calculation of the anisotropic probabilities, which depend on the form of the f and $\hat{f}$ functions. As discussed before, to meet the "integrability conditions" for the usual P_{ij}^{kl}, the f_i^k must be a polynomial in ξ^s of degree k, with $s = 1$ in plane geometry and $s = 2$ otherwise; this choice also means that the integral over ξ in Eq. (149) may be done analytically. From Eq. (146) it can be seen that $\hat{f}_j^l$ is of the form of ξ times a polynomial in ξ^s of degree l plus a term proportional to $\xi^{-\alpha}$. Use of this $\hat{f}$ in Eq. (149) permits an analytic integration over ξ' in plane geometry, but not in cylindrical and spherical geometries. In the latter cases it is necessary either to make some approximation or to use a numerical quadrature for the integral containing the $\xi^{-\alpha}$ terms.[120,131-134,136]

The anisotropic probabilities $\hat{P}$ do not obey direct symmetry relations in nonplane geometries, so that both $\hat{P}_{ij}^{kl}$ and $\hat{P}_{ji}^{lk}$ must be calculated. However, for a white boundary condition, Eqs. (117), (119), (123), and (124) can be extended to the anisotropic probabilities.[132]

III.E. Integral Transform/Spatial Spherical Harmonics Method

Convergence of the flux in the CP method is accomplished by increasing the number of spatial zones while using a constant number of expansion functions per zone. In the case of a homogeneous medium, a more attractive scheme can be constructed by using only one zone for the entire medium and expanding the flux in an ever-increasing number of expansion functions. For one-dimensional geometries, this scheme provides a very accurate and fast technique.

Multimode expansions in the spatial variable have been developed by two independent approaches. The first, formerly called the J_N method[137-140] and now more commonly known as the integral transform

[136]H. TAKAHASHI, *Nucl. Sci. Eng.*, **24**, 60 (1966).

[137]T. ASAOKA, Y. NAKAHARA, and K. SAITO, *J. Nucl. Energy A/B*, **18**, 665 (1964).

[138]T. ASAOKA, *J. Nucl. Energy*, **22**, 99 (1968).

[139]T. ASAOKA, *Nucl. Sci. Eng.*, **34**, 122 (1968).

[140]T. ASAOKA and E. C. BONANNI, *J. Nucl. Energy*, **26**, 605 (1972).

(IT_N) method,[141-150] is based on a biorthogonal expansion of the kernel of the Fourier-transformed integral operator. The second approach, which utilizes an expansion of the flux in spatial spherical harmonics,[151,152] has been shown to be formally equivalent to the IT_N method.[153]

Both approaches are projection methods. The IT_N method is, in essence, a projection technique applied to the Fourier-transformed integral transport equation; on the other hand, the spatial harmonics approach uses a straightforward projection technique to solve the usual integral transport equation. Since both approaches are currently used in the literature, we treat them separately, and consider first the IT_N method.

III.E.1. Isotropic Scattering

For simplicity we first consider the case of isotropic scattering and sources. For a homogeneous body, the transport kernel of Eq. (107) becomes a convolution kernel

$$g(\boldsymbol{r}' \to \boldsymbol{r}) = g(r) = (4\pi r^2)^{-1} \exp(-\Sigma r) \ ,$$

where $r = |\boldsymbol{r}' - \boldsymbol{r}|$ and Σ is the constant total cross section. With the definition of the convolution product

$$f_1 * f_2 = c^{-1} \int_\infty f_1(\boldsymbol{r} - \boldsymbol{r}') f_2(\boldsymbol{r}') d\boldsymbol{r}' \ ,$$

where $c = (2\pi)^{3/2}$, the Peierls Eq. (109) becomes

$$\phi = cg * (\theta F) \ . \tag{150}$$

The domain of integration has been extended to infinity by assuming that the medium is uniform everywhere. Furthermore, the solution is constrained to the initial domain D by use of the discontinuous function

$$\theta = \begin{cases} 1 \ , & \boldsymbol{r} \in D \\ 0 \ , & \text{otherwise} \end{cases} \ .$$

The next step is to apply the Fourier transform to convolution Eq. (150). With the definition

$$f^t(\boldsymbol{b}) = c^{-1} \int f(\boldsymbol{r}) \exp(-i\boldsymbol{b}\cdot\boldsymbol{r}) d\boldsymbol{r} \ ,$$

where the superscript t denotes transformed functions, we obtain

$$\phi^t = cg^t(\theta^t * F^t) \ . \tag{151}$$

Here use has been made of the identities

$$(f_1 * f_2)^t = f_1^t f_2^t$$

and

$$(f_1 f_2)^t = f_1^t * f_2^t \ .$$

To proceed further we assume that the kernel of the convolution operator θ^t* admits a biorthogonal expansion of the form

$$\theta^t(\boldsymbol{b} - \boldsymbol{b}') = V^{-1} \sum_k \chi_k(\boldsymbol{b}) \chi_k^\dagger(\boldsymbol{b}') \ .$$

(The reader should note that, in contrast to our earlier convention, *subscripts* are now used to distinguish between functions in the *single* zone.) Here V is the volume of the body, and the superscript dagger denotes the complex conjugate. Moreover, we assume that the family of functions $\{\chi_k\}$ is complete, and that they are orthogonal such that

$$(\chi_k, \chi_l) = \int_\infty \chi_k^\dagger(\boldsymbol{b}) \chi_l(\boldsymbol{b}) d\boldsymbol{b} = V\delta_{kl} \ . \tag{152}$$

The IT_N method is obtained by applying the projection technique on the subspace E_N of functions subtended by $\{\chi_k, k = 1 \text{ to } N\}$. The transformed flux is expanded as

$$\phi^t = \sum_{k \le N} \phi_k \chi_k \tag{153}$$

and, after use in Eq. (151), the result is projected onto $\{\chi_k^\dagger, k = 1 \text{ to } N\}$. This yields

$$\phi_k = V \sum_l P_{kl} F_l \ , \quad k = 1 \text{ to } N \ , \tag{154}$$

where the components of the emission density are

$$F_l = V^{-1} \int_\infty \chi_l^\dagger(\boldsymbol{b}) F^t(\boldsymbol{b}) d\boldsymbol{b} = \Sigma_s \phi_l + S_{tl} \ ,$$

and the matrix coefficients are

$$P_{kl} = cV^{-2} \int_\infty \chi_k^\dagger(\boldsymbol{b}) g^t(\boldsymbol{b}) \chi_l(\boldsymbol{b}) d\boldsymbol{b} \ . \tag{155}$$

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[141]V. C. BOFFI and V. G. MOLINARI, "Heterogeneous Methods in Neutron Transport Theory," RT/FI(68)30, Comitato Nazionale Energia Nucleare, Rome (1968).

[142]H. KSCHWENDT, *Nucl. Sci. Eng.*, **36**, 447 (1969).

[143]H. HEMBD, *Nucl. Sci. Eng.*, **40**, 224 (1970).

[144]D. C. SAHNI, *J. Nucl. Energy*, **26**, 367 (1972).

[145]H. HEMBD and H. KSCHWENDT, *J. Comp. Phys.*, **10**, 534 (1972).

[146]M. ČOPIČ, *Nucl. Sci. Eng.*, **49**, 370 (1972).

[147]A. M. MELANDRI, F. PREMUDA, and G. P. PRELATI, *Nucl. Sci. Eng.*, **55**, 225 (1974).

[148]R. SANCHEZ, "Généralisation de la Méthode d'Asaoka pour le Traitement d'une Loi de Choc Linéairement Anisotrope: Donnéés de Référence en Géometrie Cylindrique," CEA N-1831, Commissariat à l'Energie Atomique (1975).

[149]F. PREMUDA and T. TROMBETTI, *Quart. J. Mech. App. Math.*, **29**, 101 (1976).

[150]V. C. BOFFI, V. G. MOLINARI, and G. SPIGA, *Nucl. Sci. Eng.*, **62**, 332 (1977).

[151]I. CARLVIK, *Nucl. Sci. Eng.*, **31**, 295 (1968).

[152]E. B. DAHL and N. G. SJÖSTRAND, *Nucl. Sci. Eng.*, **69**, 114 (1979).

[153]J. MIKA and R. STANKIEWICZ, *Nucl. Sci. Eng.*, **36**, 450 (1969).

Let us now consider the problem of obtaining the biorthogonal expansion for the kernel $\theta^t(\boldsymbol{b} - \boldsymbol{b}')$. This problem is equivalent to solving the eigenvalue problem $\theta^t * \chi_k = \lambda_k \chi_k$, which has a solution because the operator $\theta^t *$ is compact.[153] An inverse Fourier transform of this equation yields the eigenvalue equation $\theta f_k = \lambda_k f_k$, with $\chi_k = f_k^t$. The only possible solutions of this equation are those corresponding to $\lambda_k = 0$ or $\lambda_k = 1$. In the first case the eigenfunctions are those functions which vanish in D, whereas in the second case the eigenfunctions are those functions which vanish outside D. Since the Fourier transform of an eigenfunction corresponding to $\lambda_k = 0$ belongs to the kernel of the operator $\theta^t *$, the solution of the problem is obtained by constructing a complete family of functions $\{f_k\}$ which vanish outside D. Furthermore, to obtain the normalization condition Eq. (152) we must orthonormalize the f_k by

$$\int f_k(\boldsymbol{r}) f_l(\boldsymbol{r}) d\boldsymbol{r} = V \delta_{kl} \ .$$

At this point one might wonder whether it would be possible to use the $\{f_k\}$ to directly expand the flux without any Fourier transformation. In fact, this is the basic idea of the spatial spherical harmonics (SSH_N) method, which is similar to a CP method for a single zone. The multifunction expansion for the flux takes the form

$$\phi = \sum_{k \leq N} \phi_k f_k \ . \tag{156}$$

With a similar expansion for the source, application of the projection technique to the Peierls Eq. (150) yields an equation similar to Eq. (154); now, however,

$$P_{kl} = V^{-2} \int f_k(\boldsymbol{r}) d\boldsymbol{r} \int g(\boldsymbol{r}' \to \boldsymbol{r}) f_l(\boldsymbol{r}') d\boldsymbol{r}' \ . \tag{157}$$

The IT_N and the SSH_N methods are equivalent for the case when $\chi_k = f_k^t$. Indeed, use of Parseval's formula

$$\int_\infty f_1^\dagger(\boldsymbol{r}) f_2(\boldsymbol{r}) d\boldsymbol{r} = \int_\infty [f_1^t(\boldsymbol{b})]^\dagger f_2^t(\boldsymbol{b}) d\boldsymbol{b}$$

shows that the P_{kl} in Eqs. (155) and (157) are identical, so the coefficients ϕ_k, $k = 1$ to N will be the same in both methods. Therefore, the IT_N solution Eq. (153) is just the Fourier transform of the SSH_N solution (156).

The P_{kl} satisfy the reciprocity relation $P_{kl} = P_{lk}$. Furthermore, for an isotropic surface condition, conservation relations Eqs. (123) and (124) are also valid.

Both the IT_N and SSH_N methods often have been applied to one-dimensional geometries. In the SSH_N approach, the f_k spatial modes are Legendre polynomials in plane geometry,[151] and Legendre polynomials in terms of the square of the radius in cylindrical geometry.[148] (Note that this choice is in agreement with the integrability requirements discussed in Sec. III.C for the multifunction expansions.) For both cases, the Legendre polynomial recursion relation leads to a recursion relation for the P_{kl}. For the IT_N method, the Fourier transform of these polynomials is used for the expansion functions $\chi(\boldsymbol{b})$; the calculation of the P_{kl} using Eq. (155) is obtained in terms of a rapidly converging expansion.[143]

The problem for a homogeneous sphere can be reduced to an equivalent plane geometry problem. Indeed, the spherical geometry kernel of the Peierls equation can be obtained in terms of plane geometry kernels as

$$g_2(\xi' \to \xi) = (\xi\xi')^{-1}[g_0(\xi' \to \xi) - g_0(-\xi' \to \xi)] \ .$$

Then the transport problem for the flux $\phi^s(\xi)$ in a sphere of radius a can be viewed as an equivalent problem in a slab $(-a,a)$ for the antisymmetric flux $\phi(\xi) = \xi\phi^s(\xi)$, with an antisymmetric source defined in a similar way. Consequently, the spherical case can be treated with the plane geometry formulation using only odd f_k functions.

The IT_N and SSH_N methods also have been applied to two- and three-dimensional problems,[144,154] and to the multilayer plane geometry,[140] and have produced accurate calculations for the one-dimensional critical and albedo problems.[148] In plane geometry, anisotropic scattering situations have been analyzed, and all the anisotropic matrix coefficients can be obtained from the isotropic coefficients via recursion relations.[145]

III.E.2. Linearly Anisotropic Scattering

The same reduction can be done for the three homogeneous one-dimensional geometries in the case of linearly anisotropic scattering. For simplicity, only the symmetric slab will be considered so that for the three geometries the net current vanishes at the origin. Adopting the viewpoint of the SSH_N approach, which is similar to a CP method for a single homogeneous zone, we can rewrite Eq. (148) by suppressing the summation over zones,

$$\phi_k = V \sum_l (P_{kl} F_l + \hat{P}_{kl} \hat{F}_l) \ , \quad k = 1 \text{ to } N \ . \tag{158}$$

(Observe that in agreement with the notation of this section, we have written P_{11}^{kl} as P_{kl}, with similar changes for ϕ_1^k and F_1^k, etc.) This equation has been simplified by observing that with $J(0) = 0$, the term

[154] A. BASSINI, F. PREMUDA, and W. A. WASSEF, *Nucl. Sci. Eng.*, **71**, 87 (1979).

C_1^0 in Eq. (147) vanishes so that $\hat{F}_1^0 = 0$; also, the surface contribution from Eq. (148) has been omitted.

To calculate the $\hat{P}_{kl}$, we specialize Eq. (149) to the present (single-zone) case:

$$\hat{P}_{kl} = \omega V^{-2} \int_0^a f_k(\xi)\xi^\alpha(\hat{G}_\alpha \hat{f}_l)(\xi)d\xi \ . \qquad (159)$$

Here the integration over ξ' has been identified with the action of the integral operator $\hat{G}_\alpha$ on $\hat{f}_l$. To evaluate this integration, it is convenient to use a relation between the isotropic and anisotropic kernels,[148]

$$\partial_{\xi'}[(\xi')^\alpha \hat{g}_\alpha(\xi' \to \xi)] = \Sigma(\xi')^\alpha g_\alpha(\xi' \to \xi) - \delta(\xi' - \xi) \ .$$

After integration by parts, we obtain

$$\hat{G}_\alpha \hat{f}_l = \Sigma G_\alpha f_l^* - f_l^* \ , \qquad (160)$$

where we have defined

$$f_l^*(\xi) = \int_\xi^a (\xi')^{-\alpha} d\xi' \int_0^{\xi'} f_l(\xi'')(\xi'')^\alpha d\xi'' \ .$$

Recalling that $\{f_k\}$ is a complete family of functions we can expand the function f_l^* as

$$f_l^* = \sum_k \lambda_{lk} f_k \ , \qquad (161)$$

where

$$\lambda_{lk} = V^{-1} \int f_l^*(\xi) f_k(\xi) d\boldsymbol{r} \ .$$

Finally the $\hat{P}_{kl}$ in Eq. (159) are calculated using Eqs. (160) and (161) to obtain

$$\hat{P}_{kl} = \Sigma \sum_m \lambda_{lm} P_{km} - \lambda_{kl} \ .$$

The usefulness of this last expression arises from the fact that, for the appropriate Legendre-spatial modes, $\lambda_{lm} = 0$ except for $m = l, l \pm 2$ in plane geometry and $m = l, l \pm 1$ in cylindrical geometry.[148] Consequently, for linearly anisotropic scattering, the IT_N/SSH_N method of order N requires calculation of the isotropic matrix, with elements P_{kl}, of order $(N + 2)$ for plane and spherical geometries and $(N + 1)$ for cylindrical geometry.

III.F. Nodal Methods

In large geometries the integral equation treatment becomes expensive because too many zones are required to obtain sufficient accuracy for the flux. Instead of abandoning the integral equation method in favor of an integrodifferential equation method, it is possible to utilize a nodal method.

The idea of a nodal method is to divide the domain into regions (or nodes) and to use an approximation to describe the transfer between nodes. Either the integral or the integrodifferential equation can be used to analyze the transport within each node; usually a node is homogeneous, but for some solution methods it can be heterogeneous. The solutions for adjacent nodes are linked by using approximate expansions for the angular fluxes entering and leaving the nodes.

In a nodal method, only the unknown fluxes local to a node are directly connected to one another. This results in a set of dense matrices, one for each node, that are connected by means of their interface values. Consequently, such a method is amenable to a node-by-node iterative solution in which the known incoming angular fluxes and the internal sources are used to calculate the outgoing angular fluxes.

A variety of numerical approximations have been used in the development of nodal methods, but here we shall consider only the interface current and the transverse nodal methods.

III.F.1. Interface Current Method

The principle of the interface current method consists of dividing a large medium into subregions or cells and using a simplified model to describe the transfer between cells.[105,155-158] Although the analysis of the transport within a single cell can be done with any solution method,[99,159,160] we limit our description of the interface current method to the CP treatment. Interface currents can be used to link the solutions in cells of optically large media. This is especially helpful for multidimensional geometries where a direct application of the CP method would

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[156]H. S. CHENG, C. T. McDANIEL and A. Leonard, "A Nodal Integral Transport Method for Calculation of Two-Dimensional Power Distributions in Non-Uniform Lattices," *Proc. New Developments in Reactor Mathematics and Applications,* Idaho Falls, Idaho, March 29-31, 1971, CONF-710302, Vol. II, p. 655, U.S. Atomic Energy Commission (1971).

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[159]R. J. PRYOR and W. E. GRAVES, "Response Matrix Method for Treating Reactor Calculations," *Proc. Conf. Mathematical Models and Computational Techniques for Analysis of Nuclear Systems,* Ann Arbor, Michigan, April 9-11, 1973, CONF-730414, Vol. II, p. VII-179, U.S. Atomic Energy Commission (1973).

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require accurate multidimensional numerical quadratures over large regions. Also, the interface current (IC) method reduces the coupling of the spatial variables, thus permitting an iterative cell-by-cell solution. This results in a reduction of the computing time necessary for the calculation of the collision matrix and for the solution of the system of equations for the fluxes.

We present this method for the case of isotropic scattering and sources. For every cell, the integral transport formalism is used to obtain two equations relating the scalar flux inside the cell $\phi(\boldsymbol{r})$ and angular flux leaving the cell $\psi_+(\boldsymbol{r}_b,\boldsymbol{\Omega})$ to the internal sources and angular flux entering the cell, $\psi_-(\boldsymbol{r}_b,\boldsymbol{\Omega})$. The equation for the flux is merely the Peierls equation with a surface source term,[158]

$$\phi = \int g(\boldsymbol{r}' \to \boldsymbol{r}) F(\boldsymbol{r}') d\boldsymbol{r}' - 4\pi \int g(\boldsymbol{r}'_b \to \boldsymbol{r})(\boldsymbol{\Omega}_s \cdot \boldsymbol{n}') \psi_-(\boldsymbol{r}'_b, \boldsymbol{\Omega}_s) dA' \ , \quad (162)$$

where $g(\boldsymbol{r}' \to \boldsymbol{r})$ is the collision kernel in Eq. (107). In these equations, the volume integrals are performed over the domain D of the cell, and the surface integrals are over its surface ∂D. The equation for the angular flux ψ_+ is merely Eq. (18) with q replaced by its isotropic form $F/4\pi$, so that

$$\psi_+ = \int_0^{s_b} \frac{e^{-\tau}}{4\pi} F(\boldsymbol{r}') ds + e^{-\tau} \psi_-(\boldsymbol{r}_b, \boldsymbol{\Omega}) \ . \quad (163)$$

To simplify the notation, we do not use cell indices, and will use an overbar symbol to indicate the corresponding quantity in the adjacent cell (as with $\overline{\psi}_\pm$ for $\psi_\pm$, etc.). The solutions in adjacent cells are linked via the incoming angular flux ψ_- which is simply the angular flux leaving the adjacent cell, $\overline{\psi}_+$. This continuity condition for the surface angular fluxes may be generalized to account for stationary surface sources, as well as for an arbitrary transmission or albedo factor $t(\boldsymbol{r}_b, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})$:

$$\psi_- = \psi_0 + \int_{2\pi-} t(\boldsymbol{r}_b, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}) \overline{\psi}_+(\boldsymbol{r}_b, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' \ . \quad (164)$$

Here the integral over $d\boldsymbol{\Omega}'$ is over all directions entering the cell.

Equations (162), (163), and (164) for all the cells form a closed system of equations. An approximate system can be obtained by a generalization of the projection technique in which separate expansions are assumed for the fluxes and the surface angular fluxes. Each cell is first subdivided in N zones, and the scalar flux is expanded in each zone as in the multifunction expansion (138). The surface of each cell is also subdivided into N_b subsurfaces, and on each subsurface a multifunction expansion is used for the angular flux,

$$\psi_\pm(\boldsymbol{r}_b, \boldsymbol{\Omega}) = \sum_{\alpha,\rho} J^\rho_{\pm,\alpha} f^\rho_{\pm,\alpha}(\boldsymbol{r}_b, \boldsymbol{\Omega}) \ . \quad (165)$$

Here $\rho = 1$ to P_α distinguishes the modes for each subsurface α. The expansion function $f^\rho_{\pm,\alpha}$ is defined on subsurface α for $\pm\boldsymbol{\Omega}\cdot\boldsymbol{n} > 0$ and is zero otherwise. As before, we adopt the normalization condition (139) for the spatial expansion functions, and also normalize the surface modes with the conditions[158]

$$\int f^\rho_{\pm,\alpha}(\boldsymbol{r}_b, \boldsymbol{\Omega}) f^\nu_{\pm,\beta}(\boldsymbol{r}_b, \boldsymbol{\Omega})(\boldsymbol{\Omega}\cdot\boldsymbol{n}) d\boldsymbol{\Omega} dA = \pm(\pi A_\alpha)^{-1} \delta_{\alpha\beta}\delta_{\rho\nu} \ ,$$

where A_α is the area of the α'th subsurface. The first expansion function is taken to be a constant, which gives $f^0_{\pm,\alpha} = (\pi A_\alpha)^{-1}$; hence, $J^0_{\pm,\alpha}$ is the total neutron current leaving (+) and entering (−) the cell through subsurface α. For this reason, the $J^\rho_{\pm,\alpha}$ may be called the IC components.

To obtain the desired approximate set of equations, the expansions for the fluxes and the surface angular fluxes are used in Eqs. (162), (163), and (164), and the resulting equations are projected onto the appropriate expansion functions. (Note that the projections on the surface modes $f^\rho_{\pm,\alpha}$ are done with the weight $\pm\boldsymbol{\Omega}\cdot\boldsymbol{n}$.) The resulting system of algebraic equations for each cell is[158]

$$\phi^k_i = \sum_{j,l} P^{kl}_{ij} V_j F^l_j + \sum_{\alpha,\rho} P^{k\rho}_{iS_\alpha} J^\rho_{-,\alpha} \ ,$$

$$J^\rho_{+,\alpha} = \sum_{i,k} P^{\rho k}_{S_\alpha i} V_i F^k_i + \sum_{\beta,\nu} P^{\rho\nu}_{S_\alpha S_\beta} J^\nu_{-,\beta} \ ,$$

and

$$J^\rho_{-,\alpha} = J^\rho_{0,\alpha} + \sum_{\bar{\beta},\nu} A^{\rho\nu}_{\alpha\bar{\beta}} \overline{J}^\nu_{+,\bar{\beta}} \quad (166)$$

for $i = 1$ to N, $k = 1$ to K_i, $\alpha = 1$ to N_b, and $\rho = 1$ to P_α. To obtain this set of equations, we have also used the appropriate expansions for the surface source ψ_0 and for the total volume source S_t. Aside from the coupling coefficients $A^{\rho\nu}_{\alpha\bar{\beta}}$ that account for the transmission or albedo factor, the third equation of set (166) is merely an indexing that relates the incoming angular surface modes $J^\rho_{-,\alpha}$ to the outgoing ones $\overline{J}^\rho_{+,\bar{\alpha}}$.

The matrix coefficients in Eq. (166) are closely related to collisionless probabilities. The first-flight collision probabilities P^{kl}_{ij} are those of Eq. (141), while the generalized surface-to-volume, escape, and transmission probabilities are given by[158]

$$P^{k\rho}_{iS_\alpha} = -4\pi V_i^{-1} \int f^k_i(\boldsymbol{r}) d\boldsymbol{r} \int g(\boldsymbol{r}'_b \to \boldsymbol{r}) \times f^\rho_{-,\alpha}(\boldsymbol{r}'_b, \boldsymbol{\Omega}_s)(\boldsymbol{\Omega}_s\cdot\boldsymbol{n}) dA' \ ,$$

$$P^{\rho k}_{S_\alpha i} = \pi A_\alpha V_i^{-1} \int f^k_i(\boldsymbol{r}) d\boldsymbol{r} \int g(\boldsymbol{r} \to \boldsymbol{r}'_b) \times f^\rho_{+,\alpha}(\boldsymbol{r}'_b, \boldsymbol{\Omega}_s)(\boldsymbol{\Omega}_s\cdot\boldsymbol{n}) dA' \ ,$$

and

$$P^{\rho\nu}_{S_\alpha S_\beta} = -4\pi^2 A_\alpha \int f^{\rho}_{+,\alpha}(\mathbf{r}_b, \mathbf{\Omega}_s)(\mathbf{\Omega}_s \cdot \mathbf{n}) dA$$

$$\times \int g(\mathbf{r}'_b \to \mathbf{r}_b) f^{\nu}_{-,\beta}(\mathbf{r}'_b, \mathbf{\Omega}_s)(\mathbf{\Omega}_s \cdot \mathbf{n}') dA' \ ,$$

respectively. The coupling coefficients are

$$A^{\rho\nu}_{\alpha\bar{\rho}} = -\pi A_\alpha \int f^{\rho}_{-,\alpha}(\mathbf{r}_b, \mathbf{\Omega})(\mathbf{\Omega} \cdot \mathbf{n})$$

$$\times \iint \bar{f}^{\nu}_{+,\bar{\beta}}(\mathbf{r}_b, \mathbf{\Omega}') t(\mathbf{r}_b, \mathbf{\Omega}' \to \mathbf{\Omega}) d\mathbf{\Omega} d\mathbf{\Omega}' dA$$

and may be directly calculated without numerical integration.

The time required for computation of the matrix coefficients is greatly reduced by use of the reciprocity relations[158]

$$P^{kl}_{ij} = P^{lk}_{ji} \ ,$$

$$P^{k\rho}_{iS_\alpha} = 4(A_\alpha)^{-1} P^{\rho k}_{S_\alpha i} \ ,$$

and

$$A_\beta P^{\rho\nu}_{S_\alpha S_\beta} = A_\alpha P^{\nu\rho}_{S_\beta S_\alpha} \ . \tag{167}$$

The form of the last two relations depends on the relationship between $f^{\rho}_{+,\alpha}$ and $f^{\rho}_{-,\alpha}$; here we have assumed

$$f^{\rho}_{+,\alpha}(\mathbf{r}_b, \mathbf{\Omega}) = f^{\rho}_{-,\alpha}(\mathbf{r}_b, -\mathbf{\Omega}) \ , \quad \mathbf{\Omega} \cdot \mathbf{n} > 0 \ .$$

The procedure described in Sec. III.A can be used to derive conservation relations for this formalism. With the volume source $S(\mathbf{r}, \mathbf{\Omega}) = (4\pi V_i)^{-1} f^k_i(\mathbf{r})$ and the definitions of collision and escape probabilities, Eq. (122) reduces to

$$P^{0k}_{Si} \equiv \sum_\alpha P^{0k}_{S_\alpha i} = \delta_{0k} - \sum_j \Sigma_j V_j P^{k0}_{ij} \ . \tag{168}$$

Likewise, the surface angular source $S(\mathbf{r}, \mathbf{\Omega}) = -(\mathbf{\Omega} \cdot \mathbf{n}) f^{\rho}_{-,\alpha}(\mathbf{r}_b, \mathbf{\Omega})$ and the definitions of escape and transmission probabilities yield

$$P^{0\rho}_{SS_\alpha} \equiv \sum_\beta P^{0\rho}_{S_\beta S_\alpha} = \delta_{0\rho} - 4A^{-1}_\alpha \sum_j \Sigma_j V_j P^{\rho 0}_{S_\alpha j} \ . \tag{169}$$

Equation (168) is a statement of conservation for neutrons emitted in zone i with spatial distribution of mode k; it gives the total escape probability P^{0k}_{Si} for uncollided neutrons as the difference of the total number of neutrons emitted minus the number suffering a first collision inside the cell. Similarly, Eq. (169) yields the conservation relation for neutrons entering the cell with angular mode ρ through subsurface S_α. When these equations are not used to reduce the number of probability calculations, they must be utilized as normalization conditions to guarantee neutron conservation.

We now consider the construction of the expansion functions. The treatment of the spatial variable simplifies if the cells are homogeneous, in which case one may use only one zone per cell. For example, an arbitrary two-dimensional geometry may be represented with homogeneous rectangular one-zone cells.[156,161-164] In general, this procedure requires the use of some prehomogenization that can be avoided if curved elements are employed.[155,157,159,165] This spatial representation has the advantage that the transport analysis within the cell is simple, but the numerical results often depend heavily on the approximation at the interfaces.

On the other hand, the spatial variable may be treated using more than one zone per cell. This minimizes or eliminates the need for homogenization of cells, and gives a scheme that is less dependent on the approximation of the angular flux at the interfaces. A composite-cell approximation, however, is highly dependent on the geometry of the cells, and requires a detailed transport calculation within the cells.[158,159]

The simplest approximation for the angular fluxes ψ_+ and ψ_- is to assume that they are isotropic (over a hemisphere) and uniform on the entire surface of the cell.[166] Such a procedure, however, is prone to inaccuracies for cells in the vicinity of strong flux gradients. Nevertheless, such an angular approximation has been combined with a cylindrical cell model to obtain economical two-dimensional transport codes.[167-169] To overcome the limitations of this

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[164] J. STEPANEK, "The *DPN* and *QPN* Surface Flux Integral Transport Method in One-Dimensional Geometries and in *x,y*-Geometry," *Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems*, Munich, Germany, April 27-29, 1981, Vol. 1, p. 51, Kernforschungszentrum Karlsruhe (1981).

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[169] A. HOFFMANN, F. JEANPIERRE, A. KAVENOKY, M. LIVOLANT, and H. LORAIN, "APOLLO: Code Multigroupe de Résolution de l'Equation du Transport pour les Neutrons Thermiques et Rapides," CEA-N-1610, Commissariat à l'Energie Atomique (1973).

approximation, more sophisticated angular flux expansions also have been developed. This has been done by subdividing a cell's surface into several subsurfaces or by using a higher order angular approximation for the ingoing and outgoing angular fluxes, or by both techniques.[155-158,162-165]

Finally, let us consider the solution of the system of algebraic Eqs. (166). A straightforward technique involves a cell-by-cell iteration for the flux components ϕ_i^k and for the IC components $J^{\rho}_{\pm,\alpha}$. Another approach utilizes the algebraic elimination of the IC components to obtain a set of equations for only the flux components[158]; the trouble with this approach, however, is that the set of equations becomes very tightly coupled, and hence is expensive to solve numerically. A better method is based on an algebraic elimination of the flux components, which gives a set of equations for the IC components. This method yields, for each cell, a set of equations for the outgoing current components in terms of the ingoing components. Since these ingoing components, in turn, are the outgoing components from the adjacent cells, the system of equations for all cells is weakly coupled and can be solved by cell-to-cell iterations.

The response matrix coupling the angular current components for a cell accounts for all collisions within the cell. To derive this matrix, we rewrite the first two equations of Eq. (166) for a cell in the matrix form

$$\boldsymbol{\phi} = \mathbf{P}\mathbf{V}\boldsymbol{F} + \mathbf{P}_{\cdot S}\boldsymbol{J}_{-}$$

and

$$\boldsymbol{J}_{+} = \mathbf{P}_{S\cdot}\mathbf{V}\boldsymbol{F} + \mathbf{P}_{SS}\boldsymbol{J}_{-} \ ,$$

where $\boldsymbol{F} = \boldsymbol{\Sigma}_{s0}\boldsymbol{\phi} + \boldsymbol{S}$. After solving for the flux from the first equation, we obtain the response matrix equation $\boldsymbol{J}_{+} = \mathbf{R}\boldsymbol{J}_{-} + \boldsymbol{S}_J$, where $\boldsymbol{S}_J$ comes from the source $\boldsymbol{S}$ and the response matrix $\mathbf{R}$ is

$$\mathbf{R} = \mathbf{P}_{SS} + \mathbf{P}_{S\cdot}\mathbf{V}[\boldsymbol{\Sigma}_{s0}(\mathbf{I} - \mathbf{P}\mathbf{V}\boldsymbol{\Sigma}_{s0})^{-1}\mathbf{P}_{\cdot S}] \ .$$

In this expression, the first term on the right side gives the uncollided contribution and the second term accounts for collisions within the cell.

The equations for the response matrix method usually are directly derived without resorting to the IC formalism.[106] A variety of techniques besides the CP method[162-170] have been used to construct the response matrices. For example, this includes diffusion theory,[171,172] Monte Carlo,[159,173] singular eigenfunctions,[31-33] and the S_N method.[174] The response matrix method is sometimes known as the transmission matrix method and, in plane geometry, is related to the doubling method.[175]

III.F.2. Transverse Nodal Method

The idea behind the transverse nodal (TN) method is to reduce a multidimensional transport problem to a coupled set of one-dimensional problems.[176-179] This is done for each node by approximating the solution with a factorized expansion and integrating over all but one of the spatial variables.

III.F.2.a. Cartesian Coordinates

To illustrate the method, we first consider an x-y Cartesian domain that has been divided into homogeneous nodes. Although the method can be derived from a purely integral equation approach, it is easier to begin with the integrodifferential equation

$$(\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} + \Sigma)\psi = q \ . \qquad (170)$$

To obtain a factorized approximation for the angular flux, we select two sets of linearly independent functions $\{f_i(x), i = 1 \text{ to } N_x\}$ and $\{g_k(y), k = 1$

[170]W. L. FILIPPONE, *Nucl. Sci. Eng.*, **52**, 23 (1973).

[171]K. AOKI and A. SHIMIZU, *J. Nucl. Sci. Technol.*, **2**, 149 (1965).

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[176]J. J. DORNING, "Modern Coarse-Mesh Methods–A Development of the '70's," *Proc. Topl. Mtg. Computational Methods in Nuclear Engineering*, Williamsburg, Virginia, April 23-25, 1979, CONF-790402, p. 3-1, American Nuclear Society (1979).

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[178]R. D. LAWRENCE and J. J. DORNING, "A Discrete Nodal Integral Transport Theory Method for Multidimensional Reactor Physics and Shielding Calculations," *Proc. Topl. Mtg. Advances in Reactor Physics and Shielding*, Sun Valley, Idaho, September 14-17, 1980, p. 840, American Nuclear Society (1980).

[179]W. F. WALTERS and R. D. O'DELL, "Nodal Methods for Discrete-Ordinates Transport Problems in (X,Y) Geometry," *Proc. Int. Topl. Mtg. Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems*, Munich, Germany, April 1981, Vol. 1, p. 115, Kernforschungszentrum Karlsruhe (1981).

to $N_y\}$ which, for convenience, we orthogonalize such that

$$\int_{-l_x/2}^{l_x/2} f_i(x)f_j(x)dx = \delta_{ij}l_x \ ,$$

and similarly for the $g_k(y)$ functions; here $\mp l_x/2$ are the left/right horizontal boundaries of the node. With these functions we can construct the angular flux within the cell using the ansatz

$$\psi(x,y,\mathbf{\Omega}) \sim \sum_{i,k} \psi_{i,k}(\mathbf{\Omega})f_i(x)g_k(y) \ . \qquad (171)$$

In practice, it is convenient to use different expansions for the angular fluxes on the boundaries. Denoting by $x_\pm$ the abscissa of the leaving (+) and entering (−) vertical sides of the node [i.e., $x_\pm = \pm(\text{sign } \Omega_x)l_x/2$, where Ω_x is the projection of $\mathbf{\Omega}$ on the x axis], we write

$$\psi(x_\pm,y,\mathbf{\Omega}) \sim \sum_k \psi_{kx_\pm}(\mathbf{\Omega})g_k(y) \ , \qquad (172)$$

with a similar expression for the $\psi(x, y_\pm,\mathbf{\Omega})$. The number of functions M_y selected for this expansion need not be the same as the number N_y used in expansion (171).

Once this expansion is introduced into the transport equation, the y variable can be eliminated by multiplying by $g_k(y)dy$ and integrating from $-l_y/2$ to $l_y/2$. This gives a one-dimensional transport equation

$$(\Omega_x\partial_x + \Sigma)\psi_k = W_k \ , \qquad (173)$$

where ψ_k is the k'th (vertical) transverse moment of the angular flux,

$$\psi_k(x,\mathbf{\Omega}) = \int_{-l_y/2}^{l_y/2} g_k(y)\psi(x,y,\mathbf{\Omega})dy \ .$$

The resulting effective source W_k is

$$W_k(x,\mathbf{\Omega}) = q_k(x,\mathbf{\Omega}) + \Omega_y\psi_{k'}(x,\mathbf{\Omega}) - \Omega_y\langle g_k\psi(x,y,\mathbf{\Omega})\rangle_y \ ,$$

where $\psi_{k'}$ is defined like ψ_k, but with g_k replaced by its derivative with respect to y, and the brackets $\langle\ \rangle$ denote the difference of the value at $y = l_y/2$ minus that at $-l_y/2$.

To calculate ψ_k, we invert the one-dimensional streaming operator in Eq. (173) to obtain the integral equation

$$\psi_k(x,\mathbf{\Omega}) = \Omega_x^{-1}\int_{x_-}^{x} W_k(x',\mathbf{\Omega})e^{-\tau}dx' + l_y\psi_{kx_-}(\mathbf{\Omega})e^{-\tau_-} \ , \qquad (174)$$

where the optical path length is

$$\tau(x',x) = \left|\frac{x-x'}{\Omega_x}\right|\Sigma$$

and $\tau_- = \tau(x_-,x)$. Because of the factorized form (171) of the angular flux, the transverse flux moment can be written as

$$\psi_k(x,\mathbf{\Omega}) \sim l_y \sum_i \psi_{ik}(\mathbf{\Omega})f_i(x) \ .$$

The coefficients ψ_{ik} are obtained by replacing this expansion in Eq. (174) and using the projection method to obtain

$$\psi_{ik}(\mathbf{\Omega}) = |\Omega_x|^{-1}l_x \sum_j P_{ij}(\Omega_x)W_{jk}(\mathbf{\Omega}) + P_{ix_-}(\Omega_x)\psi_{kx_-}(\mathbf{\Omega}) \ , \quad i = 1 \text{ to } N_x \ . \qquad (175)$$

Also, using the same expansion in Eq. (174) for $x = x_+$ yields an equation for the boundary outgoing angular flux

$$\psi_{kx_+}(\mathbf{\Omega}) = |\Omega_x|^{-1}l_x \sum_j P_{x_+j}(\Omega_x)W_{jk}(\mathbf{\Omega}) + P_{x_+x_-}(\Omega_x)\psi_{kx_-}(\mathbf{\Omega}) \ . \qquad (176)$$

The $W_{jk}(\mathbf{\Omega})$ in the preceding two equations is given by

$$W_{jk}(\mathbf{\Omega}) = q_{jk}(\mathbf{\Omega}) + \Omega_y\psi_{jk'}(\mathbf{\Omega}) - \Omega_y l_x^{-1}l_y^{-1}\langle g_k\psi_j(y,\mathbf{\Omega})\rangle_y \ .$$

We observe that the last term, the transverse leakage term, in this expression contains $\psi_{jy_\pm}(\mathbf{\Omega})$, the outgoing/incoming horizontal transverse moments of the angular flux; therefore, this term couples the x direction equations to the y direction equations that can be obtained in the same way by integrating the integrodifferential transport equation over the x variable.

The matrix coefficients in Eqs. (175) and (176), analogous to those in the IC method, are

$$P_{ij}(\Omega_x) = l_x^{-2}\int_{x_-}^{x_+} f_i(x)dx \int_{x_-}^{x} f_j(x')e^{-\tau}dx' \ ,$$

$$P_{ix_-}(\Omega_x) = P_{x_+i}(-\Omega_x) = l_x^{-1}\int_{-l_x/2}^{l_x/2} f_i(x)e^{-\tau_-}dx \ ,$$

and

$$P_{x_+x_-}(\Omega_x) = \exp[-\tau(x_+,x_-)] \ .$$

The calculation of these matrix coefficients is simplified by use of the appropriate reciprocity and conservation relations. For example, interchanging Ω_x with $-\Omega_x$ does not change τ, but changes $\tau_\pm$ to $\tau_\mp$ and $x_\pm$ to $x_\mp$; thus, the reciprocity relation $P_{ij}(\Omega_x) = P_{ji}(-\Omega_x)$ is recovered. Also, from the identity $\tau_+ + \tau_- = \tau(x_+,x_-)$, and assuming the usual case that $f_1(x)$ is a constant, we observe that

$$P_{x_+i}(\Omega_x) + P_{ix_-}(\Omega_x) = \delta_{i1}P_{x_+x_-} \ .$$

Furthermore, we note that the symmetric sum of two volumetric matrix coefficients can be written as

$$P_{ij}(\Omega_x) + P_{ji}(\Omega_x) = l_x^{-2} \int_{-l_x/2}^{l_x/2} f_i(x)dx \int_{-l_x/2}^{l_x/2} f_j(x')e^{-\tau}dx' \ .$$

To derive conservation relations, the procedure in Sec. III.A is again followed. We first integrate Eq. (173) from $-l_x/2$ to $l_x/2$ and then, with Q_k replaced by $f_i(x)$, we obtain

$$|\Omega_x|P_{x_+i}(\Omega_x) = \delta_{1x} - \Sigma l_x P_{1i}(\Omega_x) \ .$$

Similarly, with Q_k replaced by $\delta(x - x_-)$, it follows that

$$|\Omega_x|P_{ix_-}(\Omega_x) = 1 - \Sigma l_x P_{ix_-}(\Omega_x) \ .$$

If Legendre polynomials are used as the expansion functions in Eq. (171), the matrix coefficients can be obtained as linear combinations of exponential functions. Also, symmetry and antisymmetry properties for the matrix coefficients can be derived from the corresponding properties of Legendre polynomials. These features, together with the fact that the matrix coefficients are the same for all transverse modes ψ_k, $k = 1$ to N_y (and transverse boundary modes $\psi_{kx_\pm}$, $k = 1$ to M_y), reduce the amount of computation required.

We consider now the treatment of the angular variable. In the simple case of a plane geometry problem, in which there is no need for treatment of the transverse variable, both the discrete ordinates approximation and the projection method have been used.[177] Here we discuss only the solution of the two-dimensional problem by means of the discrete ordinates approximation. In this case, for each direction $\mathbf{\Omega} \in S_N$ the equations are solved iteratively node by node. For each node, the set of Eqs. (176) and its y counterpart that are coupled through the transverse leakage terms are solved to determine the moments $\psi_{kx_+}(\mathbf{\Omega})$, $k = 1$ to M_y, and $\psi_{iy_+}(\mathbf{\Omega})$, $i = 1$ to M_x, in the outgoing directions in terms of the ingoing ones and the volumetric sources. Then all the volumetric coefficients $\psi_{ik}(\mathbf{\Omega})$, $i = 1$ to N_x and $k = 1$ to N_y, are computed using these angular components in either the set of Eqs. (175) or its y counterpart.

The fact that either set can be used creates some uncertainty about which choice is preferred; a way to resolve this uncertainty is to eliminate the spatial cross-product terms and replace expansion (171) by

$$\psi(x,y,\mathbf{\Omega}) = \psi_{11}(\mathbf{\Omega}) + \sum_{i>1} \psi_{i1}(\mathbf{\Omega})f_i(x) + \sum_{k>1} \psi_{1k}(\mathbf{\Omega})g_k(y) \ . \quad (177)$$

Then the $\psi_{i1}(\mathbf{\Omega})$ are obtained from Eq. (175) with $k = 1$ and the $\psi_{1k}(\mathbf{\Omega})$ from the y counterpart. This simplification has been implemented in conjunction with a one-term expansion for the boundary angular fluxes, i.e., a spatially uniform angular flux on each side.[178] In another application of Eq. (177) in which a linear expansion was used for the volumetric angular flux and a linear approximation for the boundary angular flux, $\psi_{11}(\mathbf{\Omega})$ was computed from the conservation equation found by integrating Eq. (170) over the node, while $\psi_{12}(\mathbf{\Omega})$ and $\psi_{21}(\mathbf{\Omega})$ were computed as before.[179]

It may be noted that the volumetric expansion in Eq. (171) could have been used to calculate the boundary outgoing angular fluxes, instead of using the different expansion (172) and its y counterpart. If this would have been done, then Eq. (176) would not have been needed and continuity of the angular flux for a fixed direction would have been guaranteed. Such a procedure, however, would have required a costly matrix inversion for each node.

The computational efficiency of transverse nodal methods has been checked versus the customary finite difference discrete ordinates method. In plane geometry, nodal methods based on either discrete ordinates or piecewise polynomial expansions for the angular variable have been shown to be faster than the S_N method, with polynomial expansions being the best.[177,178] In x-y geometry, the nodal method with discrete ordinates is also superior to the S_N method, since fewer mesh cells are needed for penetration problems[178,179]; it is expected that the development of the two-dimensional nodal method with piecewise polynomial expansions will be even better than the one with the S_N method because ray effects can be eliminated.

Finally, the transverse nodal method can be straightforwardly extended to three-dimensional Cartesian geometries by integrating over two spatial variables.[176]

III.F.2.b. Curvilinear Coordinates

Transverse nodal methods have yet to be extended to curvilinear coordinates to our knowledge, but because of their promise we will sketch how this might be accomplished for the case of r-z geometry. We begin with the integrodifferential transport equation in its conservative form, as in Eq. (65), which is now

$$\left(\Omega_r \frac{1}{r}\partial_r r + \Omega_z \partial_z - \frac{1}{r}\partial_\chi \Omega_\phi + \Sigma\right)\psi = q \ , \quad (178)$$

where χ and the components of $\mathbf{\Omega}$ are defined in Table I. Expansions analogous to Eqs. (171) and (172), but now in the r and z variables, are used to approximate the flux within the node and on its boundaries. After projecting the transport equation onto $g_k(z)$, we obtain the r-dependent form

$$(\Omega_r \partial_r + \Sigma) r\psi_k(r,\mathbf{\Omega}) = rW_k(r,\mathbf{\Omega}) + \partial_\chi \Omega_\phi \psi_k(r,\mathbf{\Omega}) \ .$$

The major difference between this equation and the one in Cartesian coordinates is that the angular

redistribution term now appears as an additional source term.

As before, the streaming operator is inverted and the preceding equation is transformed into the form

$$r\psi_k(r,\mathbf{\Omega}) = \Omega_r^{-1}\int_{r_-}^{r}[r'W_k(r',\mathbf{\Omega})e^{-\tau} + (\partial_\chi\Omega_\phi\psi_k)(r',\mathbf{\Omega})]dr' + l_z r_-\psi_{kr_-}(\mathbf{\Omega})e^{-\tau_-} \quad . \tag{179}$$

Because of the additional factor r now present in the equation, we choose to normalize the expansion functions $f_i(r)$ by

$$\int_{\bar{r}-l_r/2}^{\bar{r}+l_r/2} f_i(r)f_j(r)rdr = S_r\delta_{ij} \quad ,$$

where S_r is $(2\pi)^{-1}$ times the area of the annulus of width l_r and midradius $\bar{r}$. After multiplication of Eq. (179) by $f_i(r)$ and integration on r, we obtain the analog of Eq. (175),

$$\psi_{ik}(\mathbf{\Omega}) = |\Omega_r|^{-1}S_r\sum_j [P_{ij}(\Omega_r)W_{jk}(\mathbf{\Omega}) + \tilde{P}_{ij}(\Omega_r)\partial_\chi\Omega_\phi\psi_{jk}(\mathbf{\Omega})] + P_{ir_-}(\Omega_r)r_-\psi_{kr_-}(\mathbf{\Omega}) \quad . \tag{180}$$

The analog of Eq. (176) now takes the form

$$r_+\psi_{kr_+}(\mathbf{\Omega}) = |\Omega_r|^{-1}S_r\sum_j [P_{r_+j}(\Omega_r)W_{jk}(\mathbf{\Omega}) + \tilde{P}_{r_+j}(\Omega_r)\partial_\chi\Omega_\phi\psi_{jk}(\mathbf{\Omega})] + P_{r_+r_-}(\Omega_r)r_-\psi_{kr_-}(\mathbf{\Omega}) \quad . \tag{181}$$

The matrix coefficients in Eqs. (180) and (181) now take the form

$$\tilde{P}_{ij}(\Omega_r) = S_r^{-2}\int_{r_-}^{r_+} f_i(r)dr\int_{r_-}^{r} f_k(r')e^{-\tau}dr' \quad ,$$

$$P_{ir_-}(\Omega_r) = \tilde{P}_{r_+i}(-\Omega_r) = S_i^{-1}\int_{\bar{r}-l_r/2}^{\bar{r}+l_r/2} f_i(r')e^{-\tau}dr' \quad ,$$

and

$$P_{r_+r_-} = \exp[-\tau(r_+,r_-)] \quad ,$$

and the $P_{ij}(\Omega_r)$ and $P_{r_+i}(\Omega_r)$ are homologous to the coefficients with tilde symbols, except that the integration in r' has an extra factor r'. This factor r' destroys the reciprocity relations for $P_{ij}(\Omega_r)$ and $P_{r_+i}(\Omega_r)$. Furthermore, because of the angular redistribution term, one cannot obtain a conservation equation for a fixed Ω_r; nevertheless, a "global" conservation relation linking all directions can be obtained by integrating over angle.

Discretization of the angular variable can be done by a discrete ordinates approximation or by using a piecewise polynomial expansion. In the first case, we proceed as for the finite difference method and integrate Eq. (65) over $\Delta\mathbf{\Omega}_m$ for $\mathbf{\Omega}_m \in S_N$. Then we repeat the previous steps for a particular $\mathbf{\Omega}_m$, with the difference that we replace the angle-averaged redistribution term with the approximation

$$w_m^{-1}\int_{\Delta\Omega_m} R_\Omega\,\psi d\mathbf{\Omega} \sim r^{-1}[\alpha_{m+}\psi_{m+} - \alpha_{m-}\psi_{m-}] \quad ,$$

where the notation $m\pm$ is the one in Eq. (72). The $\alpha_{m\pm}$ coefficients again are chosen as in Eqs. (73), (74), and (75) but with μ replaced by Ω_r (Refs. 50 and 61).

To obtain a closed system of equations, it is necessary to add supplementary equations linking the $\psi_{m\pm}$ fluxes to ψ_m. One possibility would be to assume linearity, so that ψ_m is the average of ψ_{m+} and ψ_{m-}, as in the classical diamond difference approximation.

If a projection method is used instead of a discrete ordinates approximation, then the expansion of the angular flux within a node is also done with respect to the angular variable. This implies that the angular components $\psi_{ik}(\mathbf{\Omega})$ in Eq. (180) can be written in terms of a set of expansion functions $h^\rho(\mathbf{\Omega})$, $\rho = 1$ to N_ω, as

$$\psi_{ik}(\mathbf{\Omega}) \sim \sum_\rho \psi_{ik}^\rho h^\rho(\mathbf{\Omega}) \quad .$$

Similar expansions also are assumed for the components $\psi_{kr\pm}(\mathbf{\Omega})$ and $\psi_{iz\pm}(\mathbf{\Omega})$ of the boundary angular fluxes, but none of the expansions need be of the same order. We take the functions $h^\rho(\mathbf{\Omega})$ to be orthonormal, and use the projection method with both Eqs. (180) and (181), for example, to obtain

$$\psi_{ik}^\rho = \sum_\nu\left\{S_r\sum_j [P_{ij}^{\rho\nu}W_{jk}^\nu + \tilde{P}_{ij}^{\rho\nu}\psi_{jk}^\nu] + P_{ir_-}^{\rho\nu}r_-\psi_{kr_-}^\nu\right\}$$

and

$$r_+\psi_{r_+i}^\rho = \sum_\nu\left\{S_r\sum_j [P_{r_+j}^{\rho\nu}W_{jk}^\nu + \tilde{P}_{r_+j}^{\rho\nu}\psi_{jk}^\nu] + P_{r_+r_-}^{\rho\nu}r_-\psi_{kr_-}^\nu\right\} \quad .$$

The matrix coefficients can be calculated as before, but by replacing the exponential, $\exp(-\tau)$, with one of the kernels

$$h^{\rho\nu}(r,r') = \int |\Omega_r|^{-1}h^\rho(\mathbf{\Omega})e^{-\tau}h^\nu(\mathbf{\Omega})d\mathbf{\Omega} \quad ,$$

$$\tilde{h}^{\rho\nu}(r,r') = \int |\Omega_r|^{-1}h^\rho(\mathbf{\Omega})e^{-\tau}\partial_\chi\Omega_\phi h^\nu(\mathbf{\Omega})d\mathbf{\Omega} \quad ,$$

or

$$h_s^{\rho\nu}(r,r') = \int h^\rho(\mathbf{\Omega})e^{-\tau}h^\nu(\mathbf{\Omega})d\mathbf{\Omega} \quad .$$

The first kernel is used for $P_{ij}^{\rho\nu}$ and $P_{r_+i}^{\rho\nu}$, the second with $\tilde{P}_{ij}^{\rho\nu}$ and $\tilde{P}_{r_+i}^{\rho\nu}$, and the third with $P_{ir_-}^{\rho\nu}$ and $P_{r_+r_-}^{\rho\nu}$. If piecewise polynomials in Ω_r and Ω_z are used for the expansion functions, the first kernel can be explicitly

written as a combination of exponential integral functions, while the third kernel is merely a combination of exponential functions; because of the factor $\partial_x \Omega_\phi h^\nu(\mathbf{\Omega})$, calculation of the second kernel probably would have to be done numerically.

IV. SURFACE-INTEGRAL EQUATION METHODS

In this method, the angular flux on the surface of a homogeneous body is obtained by numerically solving the surface integral transport Eq. (23). The flux inside the body, if desired, can be recovered in terms of the surface angular fluxes and the internal sources by solving the more complicated Eq. (22). Two numerical methods have been developed, the complementarity method (C_N) and the facile method (F_N).

In the C_N method, a projection technique is used to solve the surface integral equation. The resulting matrix elements are moments of the Green's function for the infinite homogeneous medium. Such a Green's function is calculated by a Fourier transformation of the Boltzmann equation. The C_N method has been used to solve critical and albedo problems for the three one-dimensional homogeneous geometries.[180-188]

In plane geometry the Green's function can be expanded in terms of the singular eigenfunctions, and then the F_N method is obtained by solving the resulting surface-integral equation with a collocation technique.[189-197] As opposed to the C_N method in which evaluation of the matrix elements requires considerable computer time, the corresponding F_N matrix elements are easy to calculate (a fact from which the French name derives).

IV.A. Complementarity (C_N) Method

We first consider the general equations of the method for a homogeneous convex body and then display the details of the method for plane geometry. We recall that the surface-integral equation was obtained by specializing Eq. (23) to a point $\boldsymbol{r}$ on the surface ∂D. To correctly interpret the value of the Green's function t_B at the surface, to be used in Eq. (23), we decompose t_B into the sum of the uncollided kernel t of Eq. (17) and the collided one t_c, and consider the limit as $\boldsymbol{r}$ approaches ∂D from the interior of the body. The only term that requires special care is the uncollided flux due to the angular flux on the surface. With the help of Eq. (17), this term can be written as

$$(TS_b)(x) = -\int_{\partial X} t(x' \to x)(\mathbf{\Omega}'\cdot\boldsymbol{n}')\psi(x')dx' \ ,$$

$$= e^{-\tau_-}\psi(x_b)\,\mathrm{sgn}(\mathbf{\Omega}\cdot\boldsymbol{n}_b) \ ,$$

where $x = (\boldsymbol{r},\mathbf{\Omega})$, with $\boldsymbol{r}$ inside the body, and $x_b = (\boldsymbol{r}_b,\mathbf{\Omega})$, where $\boldsymbol{r}_b$ is the point on the surface intersected by the line passing through $\boldsymbol{r}$ in direction $-\mathbf{\Omega}$. The optical distance between $\boldsymbol{r}$ and $\boldsymbol{r}_b$ is τ_-, and $\mathrm{sgn}(y)$ denotes the sign of y. In the limit as $\boldsymbol{r}$ approaches ∂D, this equation reduces to

$$TS_b = \begin{cases} \psi(x_b) \ , & \mathbf{\Omega}\cdot\boldsymbol{n} < 0 \\ e^{-\tau_-}\psi(x_b) \ , & \mathbf{\Omega}\cdot\boldsymbol{n} > 0 \ . \end{cases}$$

Two integral equations are obtained from the surface-integral equation, depending on the sign of $\mathbf{\Omega}\cdot\boldsymbol{n}$. For $\mathbf{\Omega}\cdot\boldsymbol{n} < 0$, one obtains a Fredholm equation of the first kind,

$$\int_{\partial X} t_c(x' \to x)(\mathbf{\Omega}'\cdot\boldsymbol{n}')\psi(x')dx' = Q(x) \ , \quad \text{on } \partial X_- \ ,$$

while for $\mathbf{\Omega}\cdot\boldsymbol{n} > 0$ the Fredholm equation is of the second kind,

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$$\int_{\partial X} t_c(x' \to x)(\boldsymbol{\Omega}' \cdot \boldsymbol{n}')\psi(x')dx' + \psi(x) = Q(x) + e^{-\tau - \tau_b}\psi(x_b) \ , \quad \text{on } \partial X_+ \ .$$

In both of these equations, the interior source contribution is

$$Q(x) = \int_X t_B(x' \to x)S(x')dx' \ .$$

Either one of these two equations defines the incoming surface flux in terms of the outgoing surface flux, so each one is the basis of an independent numerical approximation.

To distinguish between incoming and outgoing fluxes, we denote the outgoing flux $\psi(x)$, $\boldsymbol{\Omega} \cdot \boldsymbol{n} > 0$, by $\psi^+(x)$, $x \in \partial X_+$. We express the incoming flux by its reflection, $\psi^-(x) = \psi(R^- x)$, $x \in \partial X_+$, where opertor R^- reverses the angular direction, $R^-(\boldsymbol{r},\boldsymbol{\Omega}) = (\boldsymbol{r},-\boldsymbol{\Omega})$. [The reader should note that the $\psi^{\pm}(x)$ defined here are different from the even and odd flux components defined in Sec. II.D.] Since now both fluxes are defined on ∂X_+, it is also convenient to reduce all angular integrations to the domain $\boldsymbol{\Omega} \cdot \boldsymbol{n} > 0$.

In terms of the $\psi^{\pm}(x)$ functions, the two Fredholm integral equations may be written, respectively, as

$$G^{+-}\psi^+ = G^{--}\psi^- + Q(R^- x) \ , \quad \text{on } \partial X_+ \qquad (182)$$

and

$$(G^{++} + 1)\psi^+ = G^{-+}\psi^- + Q + e^{-\tau - \tau_b}\psi^-(R^- x_b) \ , \quad \text{on } \partial X_+ \ . \qquad (183)$$

Here the operator G^{+-} is defined as

$$G^{+-}f = \int_{\partial X_+} t_c(R^+ x' \to R^- x)f(x')dx' \ ,$$

where R^+ is the identity operator, and the operators G^{--}, G^{++}, and G^{-+} are defined similarly by the appropriate R operators.

In the C_N method, these two independent equations are solved with a projection technique. Both ψ^+ and ψ^- are expressed as finite expansions of order N,

$$\psi^{\pm} = \sum_{i=1}^{N} \psi_i^{\pm} f_i \ , \qquad (184)$$

where the expansion functions f_i are defined on ∂X_+. In the case in which ∂D consists of two independent surfaces (i.e., a finite slab or a hollow cylinder or sphere), independent expansions on each surface may be obtained by using functions that vanish either on one surface or on the other. After use of the expansions in Eq. (184) and after projection with weight $\boldsymbol{\Omega} \cdot \boldsymbol{n}$ onto the $\{f_i\}$, Eqs. (182) and (183) become

$$\sum_j G_{ij}^{+-}\psi_j^+ = \sum_j G_{ij}^{--}\psi_j^- + Q_i^- \ , \quad i = 1 \text{ to } N$$

and

$$\sum_j (G_{ij}^{++} + A_{ij})\psi_j^+ = \sum_j (G_{ij}^{-+} + B_{ij})\psi_j^- + Q_i^+ \ , \quad i = 1 \text{ to } N \ . \qquad (185)$$

The matrix coefficients and the source elements are defined in terms of the scalar product of Eq. (85) as

$$A_{ij} = \langle f_i, f_j \rangle_+ \ ,$$

$$B_{ij} = \langle f_i, e^{-\tau - \tau_b} f_j(R^- x_b) \rangle_+ \ ,$$

and

$$Q_i^{\pm} = \langle f_i, Q(R^{\pm} x) \rangle_+ \ .$$

The remaining matrix coefficients are written, for example, as

$$G_{ij}^{+-} = \langle f_i, G^{+-} f_j \rangle_+ = \int_{\partial X_+} (\boldsymbol{\Omega} \cdot \boldsymbol{n}) f_i(x)dx \times \int_{\partial X_+} (\boldsymbol{\Omega}' \cdot \boldsymbol{n}') t_c(R^+ x' \to R^- x) f_j(x')dx' \ . \qquad (186)$$

When calculating matrix coefficients, a great amount of computer time may be saved by use of the reciprocity relations

$$G_{ij}^{+-} = G_{ji}^{+-} \ , \quad G_{ij}^{-+} = G_{ji}^{-+} \ , \quad G_{ij}^{++} = G_{ji}^{--} \ ,$$

which follow from the reciprocity of the collided kernel,[4] $t_c(x' \to x) = t_c(R^- x \to R^- x')$. To calculate the remaining coefficients, one has to first derive the closed-form expression for the collided kernel. This is done by determining the infinite medium Green's function in the geometry of interest, and then by subtracting the uncollided contribution. Since the infinite-medium Green's function is translationally invariant, i.e., $t_B(x' \to x) = t_B(\boldsymbol{r}' - \boldsymbol{r}, \boldsymbol{\Omega}' \cdot \boldsymbol{\Omega})$, it can be calculated by analytically solving the Fourier-transformed transport equation, and then inverting the transform. For instance, for an azimuthally independent homogeneous plane geometry with isotropic scattering, the collided kernel takes the form[181]

$$t_c(z' - z, \mu' \to \mu) = \frac{c}{4\pi} \int_{-\infty}^{\infty} \exp[ik(z' - z)] \times \frac{dk}{ik\mu'(1 - ik\mu)(1 - ck^{-1} \tan^{-1} k)} \ . \qquad (187)$$

We can use this expression to explain the calculation of the matrix coefficients G_{ij}^{+-}, etc., in plane geometry. In this geometry the expansion functions are traditionally taken to be $f_i(\mu) = \mu^{i-1}$, $i = 1$ to N. With the last kernel, evaluation of the matrix coefficients requires integrations over μ, μ', and k. The first two integrations may be done analytically, while the integration over k is extended in the usual way to encircle the upper half of the complex plane. Then, after

applying Cauchy's theorem, the asymptotic contribution (poles) is analytically evaluated whereas the transient contribution (branch) must be calculated by numerical integration in the complex plane.

The C_N method has been applied to plane geometry problems with anisotropic scattering[187] and to cylindrical and spherical problems with isotropic scattering.[183-185,187] Although the method strictly applies to homogeneous bodies, multilayer problems can be done by treating each layer separately and imposing continuity of the angular flux at the interfaces. Even more complicated geometries (such as a "cluster cell") have been analyzed.[188]

A perspective on the potential of the C_N method for the analysis of complicated geometries can be obtained by comparison with the collision probability method. An important difference is that the CP method uses a Green's function for first-flight interactions and this requires spatial zones of the order of the neutron mean-free-path; there is no such restriction in the C_N method provided the slowing down source in each homogeneous zone can be assumed constant. Furthermore, in the C_N method only neighboring zones are connected, whereas all the zones are connected in the CP method.

IV.B. Facile (F_N) Method

This method has been initially derived from the C_N method in plane geometry by using a singular eigenfunction expansion of the Green's function.[189] The F_N method also has been independently derived,[190,191] in a more direct way, by using the completeness and orthogonality properties of the singular eigenfunctions $\phi_\nu(\mu)$. Here we follow the latter approach to illustrate use of the method for the case of a finite slab $a \leqslant z \leqslant b$ in which the scattering is isotropic. The slab is assumed to be irradiated on both surfaces, and there are no internal sources.

The first step is to obtain an equation connecting the angular fluxes on the surfaces by using the singular eigenfunction expansion for the angular flux, given in Eq. (42), where now the particular solution ψ_p vanishes. The expansion coefficients $A(\nu)$ are given in terms of the angular flux by Eq. (43). We write this equation for the surfaces $z = a$ and $z = b$ and eliminate the product $A(\nu)N(\nu)$ to obtain

$$(\phi_\nu, \psi_b - \exp[-\tau/\nu]\psi_a) = 0 \quad , \quad \nu \in \sigma \quad . \tag{188}$$

In this integral equation the scalar product is that of Eq. (41), ψ_a and ψ_b denote the angular fluxes on the surfaces, and τ is the slab optical thickness. We recall that the spectrum σ consists of the interval $-1 \leqslant \nu \leqslant 1$ and the set of discrete eigenvalues.

Equation (188) is decomposed into two equations, one for the positive spectrum σ_+ and the second for the negative spectrum. Then one takes advantage of the symmetry of the spectrum to transform the latter into an equation on σ_+. The result is

$$(\phi_\nu, \psi_b - \exp[-\tau/\nu]\psi_a) = 0 \quad , \quad \nu \in \sigma_+$$

and

$$(\phi_{-\nu}, \exp[-\tau/\nu]\psi_b - \psi_a) = 0 \quad , \quad \nu \in \sigma_+ \quad . \tag{189}$$

This pair of coupled integral equations is solved by the collocation technique. As in the C_N method, the unknown emerging angular fluxes are expanded in powers of μ,

$$\psi_a(-\mu) = \sum_{k=1}^{N} a_k \mu^{k-1} \quad , \quad 0 \leqslant \mu \leqslant 1$$

and

$$\psi_b(\mu) = \sum_{k=1}^{N} b_k \mu^{k-1} \quad , \quad 0 \leqslant \mu \leqslant 1 \quad . \tag{190}$$

However, if an incident angular distribution has a singular nature (i.e., delta function), these expansions should be modified to explicitly treat the uncollided singular contribution.[197]

After substituting expansions (190) into the integral Eqs. (189), the resulting equations are specialized to the collocation set $\sigma_N = \{\nu_i, i = 1 \text{ to } N, \nu_i \in \sigma_+\}$. This yields the system of equations

$$\sum_{j=1}^{N} [B_j(\nu)a_j + \exp(-\tau/\nu)A_j(\nu)b_j] = L_1(\nu) \quad , \quad \nu \in \sigma_N$$

and

$$\sum_{j=1}^{N} [\exp(-\tau/\nu)A_j(\nu)a_j + B_j(\nu)b_j] = L_2(\nu) \quad , \quad \nu \in \sigma_N \quad . \tag{191}$$

The source terms are defined as

$$L_1(\nu) = \sum_{j=1}^{N} [A_j(\nu)\tilde{a}_j + \exp(-\tau/\nu)B_j(\nu)\tilde{b}_j]$$

and

$$L_2(\nu) = \sum_{j=1}^{N} [\exp(-\tau/\nu)B_j(\nu)\tilde{a}_j + A_j(\nu)\tilde{b}_j] \quad ,$$

where $\tilde{a}_j$ and $\tilde{b}_j$ are the expansion coefficients for the known incoming angular fluxes $\psi_a(\mu)$ and $\psi_b(-\mu)$, $0 \leqslant \mu \leqslant 1$, as in Eq. (190). [Note that the system of Eqs. (191) also could be obtained by substituting the expansions directly into Eq. (188) and then by using a symmetric collocation set.]

Let us now consider the calculation of the matrix coefficients $A_j(\nu)$ and $B_j(\nu)$ in Eq. (191). The $B_j(\nu)$ are defined by

$$B_j(\nu) = \frac{2}{c\nu} \int_0^1 \mu^j \phi_\nu(\mu) d\mu$$

and, using the symmetry $\phi_\nu(\mu) = \phi_{-\nu}(-\mu)$, it is found that

$$A_j(\nu) = -B_j(-\nu) \ .$$

For the special case of Eq. (32) for isotropic scattering, it follows that these coefficients obey the recursion relation[189]

$$B_{j+1}(\nu) = \nu B_j(\nu) - (j+1)^{-1} \ , \quad j \geqslant 1 \ , \qquad (192)$$

with the starting conditions

$$B_1(\nu) = (2/c) - 1 - \nu \log(1 + 1/\nu) \ , \quad \nu \in \sigma_N$$

and

$$A_1(\nu) = 1 - \nu \log(1 + 1/\nu) \ , \quad \nu \in \sigma_N \ .$$

Notice that the numerical effort involved in the calculation of the matrix coefficients requires the computation of only N logarithms! Of course, the solution depends on the distribution of the collocation points, and numerical calculations show that the discrete spectrum has to be included to ensure good results.

The F_N method has been extended to treat problems with anisotropic scattering,[191] but is restricted to plane and spherical geometries, as for singular eigenfunction expansions. Multilayer problems have been solved by treating each layer separately,[195,196] and also the theory has been extended to slowing down problems.[189,195]

V. COMMENTS

The deterministic methods of solution of the transport equation are based on the use of the integrodifferential, integral, and surface-integral equations. In this paper, we have shown that the most common solution methods are based on three numerical techniques: expansion (projection and collocation) methods, quadrature formulas for integral operators, and finite differences for differential operators.

By taking advantage of the special properties of the transport operator in simple geometries, it is possible to obtain an analytical (or quasi-analytical) solution. Extensive research has been dedicated to deriving such solutions with singular eigenfunction expansions, analytic discrete ordinates, integral transform/spatial spherical harmonics, and the two surface-integral methods (C_N and F_N). The usefulness of such quasi-numerical techniques is to provide benchmark solutions to check more general numerical methods, to gain insight into the mathematical properties of the transport equation, and to provide intellectual stimulation for the analytically inclined analyst. For more realistic problems, a fully numerical treatment with one of the following general-purpose production methods is required.

The integrodifferential equation methods, those most widely studied by researchers in the U.S., have been used to solve a variety of problems in reactor and shielding analysis. The integrodifferential equation is based on a local neutron balance and contains spatial derivatives and an integral angular operator. Both the angular and spatial variables require a numerical treatment. The finite difference discrete ordinates method is characterized by the use of a numerical quadrature formula for the integral angular operator and a finite difference approximation for the spatial derivatives. Potential difficulties with the method are the appearance of negative fluxes and ray effects. Expensive modifications, usually based on the implementation of a spherical harmonics representation within the discrete ordinates formalism, have been developed to eliminate such ray effects.

Many spatial cells are required with the finite difference discrete ordinates method for treatment of large-scale reactor and shielding problems, especially when streaming is important. Without loss of precision, it is possible to use large-sized cells if the angular fluxes entering and leaving a cell are related by integration along neutron trajectories. In the method of characteristics, this integration is combined with a cell balance equation for treatment of the spatial variable, while a discrete ordinates approximation is used for the angular variable.

A variation of the discrete ordinates technique is to combine the numerical integration in the angular variable with a finite element treatment (a projection technique) for the spatial variable. Although the finite element system of equations requires more computational work, it does provide a better representation for irregularly shaped geometries. On the other hand, a complete finite element approximation for the integrodifferential equation is derived by applying the finite element method to both the angular and spatial variables. Such a full finite element treatment has been applied to the ordinary and to the even-party forms of the transport equation. The finite element approach is appealing because it mitigates the ray effects and offers a self-consistent treatment of boundary conditions, but the method is not yet economically competitive with the discrete ordinates approach.

Integral equation methods have been more popular in Europe and they are especially appropriate for cell and subassembly calculations. The integral equation is based on a global neutron balance and consequently is strongly coupled in both variables. For isotropic scattering, the angular variable is integrated out to yield an integral equation in the spatial variable for the scalar flux. Numerical quadrature techniques and expansion methods have been applied to solve the integral equation. The numerical quadrature

approach leads to the discrete integral transport method, while piecewise polynomial expansions are used to construct approximations via the collocation and the projection (collision probability) techniques. In contrast with the DIT and CP methods, the collocation technique leads to a nonsymmetric collision matrix and requires special care to ensure neutron conservation. Of the three methods, the CP method is the most widely used. Integral equation methods also have been extended to the treatment of linearly anisotropic scattering.

In general, integrodifferential methods are most appropriate for optically large media while integral methods work best for optically small media. Integral methods can be made efficient for calculations in moderately large media, however, by use of nodal methods. In these methods, a large medium is divided into nodes and a simplified model is used to describe the transfer between the nodes. The interface current method, an early nodal approach, is constructed from a generalized projective technique by expanding the angular fluxes on the surfaces and the scalar fluxes in the nodes. Also, by eliminating the scalar fluxes, the IC method yields the response matrix formalism; integrodifferential equation methods and even Monte Carlo techniques have been used in conjunction with response matrices. A recent development in nodal techniques is to reduce a multidimensional problem to coupled one-dimensional problems by integrating over all but one of the spatial variables. This is the idea behind the transverse nodal methods that can utilize either a discrete ordinates approach or a projection technique for the treatment of the angular variable.

Neutron transport solution methods have evolved from the earliest days of interest in nuclear power. The development of improved numerical techniques for the solution of the transport equation has been closely linked to that of computers. It is the rapid development of computer technology that has lead to the use of accurate transport calculations in reactor design. Thus it is understandable why some of the earlier, elegant techniques now have at best a small role for practical reactor and shielding calculations.

The trend nowadays in the development of numerical approximations is in the synergistic use of both the integrodifferential and integral forms of the transport equation. For example, work is currently under way on the method of characteristics and on transverse nodal approximations. It is expected that improvements in already-established methods, and in these new methods, will be developed to match the capability of faster and larger computers of the future. It is safe to assume that within the next few years all of the transport approximations will have to be re-evaluated for use with parallel-processing computers.

APPENDIX

ITERATIVE SOLUTION OF THE MULTIGROUP EQUATIONS

Any practical application of numerical solution of the transport equation is based on the use of a multigroup formalism. As a complement to the discussion of one-group numerical methods, in this Appendix we give a brief description of the iterative techniques and acceleration schemes currently used for the solution of the multigroup equations.

Integrodifferential Equation Methods

We assume the reader is familiar with the multigroup formalism and we write the set of multigroup integrodifferential equations in the form

$$\mathbf{L}\boldsymbol{\psi} = \mathbf{H}\boldsymbol{\psi} + \boldsymbol{S} \ , \tag{A.1}$$

where

$\boldsymbol{\psi}$ = vector whose elements are $\{\psi_g(\boldsymbol{r},\boldsymbol{\Omega}),\ g = 1 \text{ to } G\}$

$\boldsymbol{S}$ = external source vector

$\mathbf{L}$ = diagonal matrix operator whose elements are

$$L_{gg} = \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} + \Sigma_g(\boldsymbol{r}) \ ,$$

$\mathbf{H}$ = matrix operator with elements $H_{gg'}$ so that

$$H_{gg'}f = \int \Sigma_{g'\to g}(\boldsymbol{r},\boldsymbol{\Omega}' \to \boldsymbol{\Omega}) f(\boldsymbol{\Omega}')\, d\boldsymbol{\Omega}' \ . \tag{A.2}$$

In the multigroup case, $\Sigma_{g'\to g}$ accounts for all neutrons in group g, generated by a collision or fission in energy group g', namely,

$$\Sigma_{g'\to g} = \Sigma_{s,g'\to g} + (4\pi)^{-1}(\nu\Sigma_f)_{g'}\chi_g \ .$$

[For simplicity, we have neglected $(n,2n)$ and other such reactions.]

For any numerical method, the $\psi_g(\boldsymbol{r},\boldsymbol{\Omega})$ are replaced by the values of the flux at all mesh points in space and angle, and the operators $\mathbf{L}$ and $\mathbf{H}$ in Eq. (A.1) are replaced by the appropriate matrices. The direct solution of any such matrix equation by inversion of matrix $(\mathbf{L} - \mathbf{H})$ is unfeasible and uneconomical. Therefore a dual iteration strategy is implemented, consisting of two nested iterations: an outer and an inner iteration. An outer iteration sweeps through all energy groups, in order of decreasing energy, and provides an updated value of the flux for the entire system. This is done by splitting the matrix $\mathbf{H}$ into four parts, the (in-group) self-scattering ($\mathbf{H}^s$) portion, the upscattering ($\mathbf{H}^u$) and downscattering ($\mathbf{H}^d$) parts, and the fission portion ($\mathbf{H}^f$), and defining the outer iterative scheme by

$$(\mathbf{L} - \mathbf{H}^d - \mathbf{H}^s)\boldsymbol{\psi}^n = (\mathbf{H}^u + \mathbf{H}^f)\boldsymbol{\psi}^{n-1} + \boldsymbol{S} \ . \tag{A.3}$$

That is, at the beginning of an outer iteration, the old flux ψ^{n-1} is used to calculate the upscattering and fission contributions, and then the new flux ψ^n is calculated by solving this last equation group-by-group.

The presence of the self-scattering term in Eq. (A.3) makes direct inversion of the matrix $(\mathbf{L} - \mathbf{H}^d - \mathbf{H}^s)$ impractical, so in discrete ordinates methods the following inner iteration procedure is adopted:

$$\mathbf{L}_{gg}\psi_g^{n,k} = \mathbf{H}_{gg}^s\psi_g^{n,k-1} + Q_g^n \quad . \tag{A.4}$$

Here $\psi_g^{n,k}$ is a vector whose components are values of the angular flux in group g for the space and angular mesh for outer iteration n and inner iteration k, and Q_g^n is the effective within-group source

$$Q_g^n = [\mathbf{H}^d\psi^n + (\mathbf{H}^u + \mathbf{H}^f)\psi^{n-1} + S]_g \quad .$$

This source is calculated with the most recently available fluxes, which means that the downscattering term uses fluxes from the current outer iteration, while the upscattering and fission contributions are computed from the flux in the previous outer iteration. That is, using the effective source and the previous estimate for the within group flux, $\psi_g^{n,k-1}$, an inner iteration requires sweeping through all the directions and regions to calculate from Eq. (A.4) the updated flux $\psi_g^{n,k}$.

Convergence of an iteration procedure can be assessed by imposing convergence criteria. A variety of criteria are used, but usually for inner iterations one requires that the relative error in the scalar flux for two successive iterates be less than a prescribed small value. Another procedure that is adopted is to stop the number of iterations at a prescribed number, even though convergence may not have been achieved; this is particularly advantageous for the first few outer iterations, for which complete convergence of inner iterations is expensive and does not appreciably improve the overall rate of convergence.

In the case of a calculation for the effective multiplication factor λ, there is no external source and Eq. (A.1) is replaced by

$$\mathbf{L}\psi = (\mathbf{H}^u + \mathbf{H}^s + \mathbf{H}^d)\psi + \lambda^{-1}\mathbf{H}^f\psi \quad .$$

An estimation of λ can be obtained from two successive outer iterations as the ratio of the corresponding fission sources

$$\lambda^n = \sum_g \int_D (\nu\Sigma_f)_g \psi_g^n d\boldsymbol{r} \Big/ \sum_g \int_D (\nu\Sigma_f)_g \psi_g^{n-1} d\boldsymbol{r}$$

and the outer iteration is terminated when the relative error between two successive eigenvalues is sufficiently small.

Solving the set of Eqs. (A.4) in the direction of neutron flow usually ensures that the solution is stable and allows implementation of a strategy for which matrix $\mathbf{L}_{gg}$ is lower triangular. Nevertheless, many iterations may be required to obtain a converged solution. This is especially true for optically thick regions in which the term $\mathbf{H}_{gg}^s\psi_g^{n,k-1}$ in Eq. (A.4) strongly affects the solution. For this reason, all practical numerical techniques require the use of an acceleration scheme. Chebyshev acceleration[198] has been successfully implemented in one-dimensional discrete ordinates codes,[68,199] while coarse-mesh rebalancing and the synthetic method are used in two-dimensional discrete ordinate codes.

Methods that use a discrete ordinates approximation for the angular variable and finite elements for the spatial variable utilize similar acceleration methods to those currently used in finite difference codes.[89,93,94,103] On the other hand, a finite element approximation in both the angular and spatial variables (such as those used to solve the even-parity form of the transport equation) cannot be solved by a simple cell-to-cell iteration scheme because of the coupling in space and angle. In this case, an iterative solution is obtained by such classical techniques as block (or point) successive overrelaxation[198]; usually a Cholesky decomposition is used to invert the main block, and the banded structure of the matrix is exploited to minimize computer requirements.[86,97,102] Block overrelaxation also has been accelerated with the rebalancing method.[102]

In this Appendix, we discuss only the rebalancing and synthetic methods, and refer the reader to Varga[198] for the more classical techniques.

Rebalancing Methods

Rebalancing is a popular scheme applied to production codes to accelerate inner and outer iterations.[61,69] The objective of a rebalancing scheme is to enhance the rate of convergence by imposing neutron conservation after every iteration. There are several schemes based on rebalancing, but we first discuss the method for coarse-mesh rebalancing of inner iterations.

The need for rebalancing becomes obvious when we examine the balance equation derived by integrating the iterative scheme of Eq. (A.4) over a coarse-mesh region D_α and all angular directions to obtain

$$\int_{\partial D_\alpha} \boldsymbol{J}_g^{n,k} \cdot d\boldsymbol{A} = \int_{D_\alpha} (Q_{tg}^n - \Sigma_{ag}\phi_g^{n,k-1}) d\boldsymbol{r} \quad , \tag{A.5}$$

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[198] R. S. VARGA, *Matrix Iterative Analysis*, Prentice-Hall Publishing Company, Englewood Cliffs, New Jersey (1962).

[199] E. M. GELBARD, J. A. DAVIS, and L. A. HAGEMAN, "Solution of the Discrete Ordinate Equations in One and Two Dimensions," *Proc. Applied Mathematics, Vol. 1, Transport Theory*, p. 129, American Mathematical Society, Providence, Rhode Island (1969).

where

Q_{tg}^n = total volumetric source obtained by integrating Q_g^n over all angles

Σ_{ag} = effective absorption (i.e., removal) cross section $\Sigma_{ag} = \Sigma_g - \Sigma_{s0,g\to g}$,

and the current and scalar flux are determined from the angular fluxes by applying the usual S_N rule. Neutron balance would require that $Q_g^{n,k-1}$ be replaced by $Q_g^{n,k}$, which will occur only when the iteration converges.

In the coarse-mesh rebalancing scheme, the entire domain is divided into a set of coarse-mesh regions $\{D_\alpha\}$ and neutron balance is imposed by multiplying the flux within each region α by a constant scaling factor C_α. These constants are determined from the system of equations

$$C_\alpha \left[\int_{\partial D_\alpha} \boldsymbol{J}_{+,g}^{n,k} \cdot d\boldsymbol{A} + \int_{D_\alpha} \Sigma_{ag} \phi_g^{n,k} d\boldsymbol{r} \right] + \sum_\beta C_\beta \int_{\partial D_{\alpha\beta}} \boldsymbol{J}_{-,g}^{n,k} \cdot d\boldsymbol{A} = \int_{D_\alpha} Q_{tg}^n d\boldsymbol{r} \qquad \text{(A.6)}$$

that are nothing else than the conservation equations for the modified fluxes $C_\alpha \psi_g(\boldsymbol{r},\boldsymbol{\Omega})$ in each D_α. Note that since the angular fluxes in adjacent coarse-mesh regions with a common boundary $\partial D_{\alpha\beta}$ are multiplied by different factors, it is necessary to split the current into the leaving current $\boldsymbol{J}_+$ and the entering $\boldsymbol{J}_-$. Usually acceleration of the inner iterations by application of the rebalancing factors quickly brings all flux amplitudes close to their converged values, so only a few additional iterations are needed to refine the flux shape.

The first application of rebalancing to inner iterations utilized the global scheme for which all fluxes in the entire domain were multiplied by the same constant[200]; nowadays, the general coarse-mesh rebalancing is applied, with the possibility of even using the fine mesh used to calculate the fluxes.[61,69,93,94] Another rebalancing scheme that has been examined uses a coarse-mesh angle-dependent rebalancing in both the space and angular variables. In this case the angular region is also divided into coarse regions and a balance equation similar to Eq. (A.5) is obtained by integration over a spatial and an angular region; then neutron conservation is forced by multiplying all the fluxes in a given spatial and angular region by the same factor.[54]

Still another rebalancing scheme is based on a variational principle in which a scaling function of the form

$$\sum_\alpha C_\alpha f_\alpha(\boldsymbol{r})$$

is utilized.[201] Here the $f_\alpha(\boldsymbol{r})$ are "finite elements" defined on a coarse mesh and the expansion coefficients C_α are calculated by using a weighted residual or a finite element method.

Coarse-mesh rebalancing is also applied to acceleration of outer iterations. In this case, the rebalancing constants are determined from a balance equation obtained by collapsing all the energy groups into one[61,69,93,94] and scaling all the group angular fluxes within a coarse-mesh region α with the same constant C_α. These constants are determined from a set of equations similar to set (A.6),

$$C_\alpha \sum_g \left[\int_{\partial D_\alpha} \boldsymbol{J}_{+,g}^n \cdot d\boldsymbol{A} - \int_{D_\alpha} (c_g - 1)\Sigma_g \phi_g^n d\boldsymbol{r} \right] + \sum_\beta C_\beta \sum_g \int_{\partial D_{\alpha\beta}} \boldsymbol{J}_{-,g}^n \cdot d\boldsymbol{A} = \sum_g \int_{D_\alpha} S_{tg} d\boldsymbol{r} \ ,$$

where c_g is defined as the mean number of secondaries for collisions in group g,

$$c_g = \left[(\nu\Sigma_f)_g + \sum_{g'} \Sigma_{s0,g\to g'} \right] \Big/ \Sigma_g \ .$$

Another method for rebalancing the outer iterations has been suggested in which a global neutron balance is imposed separately for every group.[202] The scaling coefficients C_g for each group g are then obtained from the equations

$$C_g \left\{ \int_{\partial D} \boldsymbol{J}_g^n \cdot d\boldsymbol{A} + \int_D [\Sigma_{ag} - \chi_g(\nu\Sigma_f)_g] \phi_g d\boldsymbol{r} \right\} = \sum_{g' \neq g} C_{g'} \int_D [\Sigma_{s0,g'\to g} + \chi_g(\nu\Sigma_f)_{g'}] \phi_{g'} d\boldsymbol{r} + \int_D S_{tg} d\boldsymbol{r} \ .$$

Synthetic Methods

The idea of a synthetic method is to use a lower order approximation to accelerate the rate of convergence of a higher order one. We will again illustrate the idea of the method by considering its use for an inner iteration procedure [Eq. (A.4)]. For convenience we drop all unnecessary indices and write the equation as

$$\mathbf{L}\psi^k = \mathbf{H}\psi^{k-1} + \boldsymbol{Q} \ . \qquad \text{(A.7)}$$

We first observe that at any stage of the iteration the exact solution ψ can be obtained from the relation[203]

$$\psi = \psi^k + (\mathbf{L} - \mathbf{H})^{-1}\mathbf{H}\delta\psi^k \ , \qquad \text{(A.8)}$$

[200]B. G. CARLSON and G. I. BELL, *Proc. Second Int. Conf. Peaceful Uses of Atomic Energy*, Geneva, Switzerland, September 1-13, 1958, Vol. 16, p. 535, United Nations, New York (1955).

[201]S. NAKAMURA, *Nucl. Sci. Eng.*, **39**, 278 (1970).

[202]B. E. CLANCY and I. J. DONNELLY, *Nucl. Sci. Eng.*, **39**, 398 (1970).

[203]W. H. REED, *Nucl. Sci. Eng.*, **45**, 245 (1971).

where the difference between two successive iterates is

$$\delta\psi^k = \psi^k - \psi^{k-1} \ .$$

Direct use of Eq. (A.8) would entail the inversion of $(\mathbf{L} - \mathbf{H})$ and would constitute the very operation we are trying to avoid with the iteration procedure. Nevertheless, the relation in Eq. (A.8) can still be used if we use a "lower order" equation

$$\mathbf{L}_l\psi = \mathbf{H}_l\psi + \mathbf{Q}$$

and replace $(\mathbf{L} - \mathbf{H})^{-1}$ in Eq. (A.8) by the inverse operator $(\mathbf{L}_l - \mathbf{H}_l)^{-1}$ that is less expensive (or easier) to calculate. As an example, a transport operator could be replaced by a diffusion operator.

The entire procedure consists of using Eq. (A.7) to obtain an intermediate vector ψ^k, and then substituting this vector into Eq. (A.8), with the lower inverse, to obtain the final ψ^k as

$$\psi^k = [\mathbf{I} - (\mathbf{L}_l - \mathbf{H}_l)^{-1}(\mathbf{L} - \mathbf{H})]\mathbf{L}^{-1}\mathbf{H}\psi^{k-1} + [\mathbf{I} + (\mathbf{L}_l - \mathbf{H}_l)^{-1}\mathbf{H}]\mathbf{L}^{-1}\mathbf{Q} \ .$$

Low-order S_N calculations have been used to accelerate higher order S_N calculations,[204] and diffusion theory solutions also have been applied to accelerate S_N calculations with finite difference approximations[204] and characteristic methods.[71]

The rebalancing and synthetic acceleration methods are closely related. In fact, rebalancing can be viewed as a synthetic method in which the lower order approximation is changed at every iteration.[203]

Integral Equation Methods

Since an integral equation method typically is used in smaller geometries than integrodifferential equation methods, the size of the matrices tends to be smaller. Therefore the numerical burden imposed by the solution of the equations is less acute than for integrodifferential equation methods for which the inversion takes the major portion of the calculation time.

Here we shall only illustrate the case of the multigroup integral equation with isotropic scattering and sources,

$$\boldsymbol{\phi} = \mathbf{G}(\mathbf{H}_t\boldsymbol{\phi} + \boldsymbol{S}_t) \ , \qquad \text{(A.9)}$$

where $\mathbf{G}$ is a diagonal matrix operator with elements G_{gg} so that

$$G_{gg}f = \int_D \frac{\exp(-\tau_g)}{4\pi s^2} f(\mathbf{r}')d\mathbf{r}' \ .$$

The matrix $\mathbf{H}_t$, which is related to the integral over all directions of operator $\mathbf{H}$ in Eq. (A.2) for isotropic scattering, has the elements

$$H_{t,gg'} = \Sigma_{s0,g'\to g} + (\nu\Sigma_f)_{g'}\chi_g \ ,$$

and $\boldsymbol{S}_t$ is the total volumetric source.

For the numerical solution, the operators in Eq. (A.9) are replaced by matrices and then $\boldsymbol{\phi}$ becomes a vector whose components are the fluxes for all the energy groups and spatial zones. The matrix $\mathbf{H}$ is decomposed into up-, in-, and down-group scattering and fission, as in Eq. (A.3), and Eq. (A.9) is solved by the outer iteration scheme

$$\boldsymbol{\phi}^n = \mathbf{G}[(\mathbf{H}_t^d + \mathbf{H}_t^s)\boldsymbol{\phi}^n + (\mathbf{H}_t^u + \mathbf{H}_t^f)\boldsymbol{\phi}^{n-1} + \boldsymbol{S}_t] \ . \qquad \text{(A.10)}$$

Again this equation is solved group by group, in the order of decreasing energies, which requires the solution for each group of the following source problem:

$$\phi_g^n = G_{gg}\Sigma_{s0,g\to g}\phi_g^n + Q_{t,g}^n \ , \qquad \text{(A.11)}$$

where $Q_{t,g}$ is the uncollided term originating from the angle-integrated effective within-group source,

$$Q_{t,g}^n = G_{gg}\left[\sum_{g'>g}\Sigma_{s0,g'\to g}\phi_{g'}^n + \sum_{g'<g}\Sigma_{s0,g'\to g}\phi_{g'}^{n-1} + \chi_g\sum_{g'}(\nu\Sigma_f)_{g'}\phi_{g'}^{n-1} + S_{t,g}\right] \ .$$

Another outer iteration scheme also has been used in which the upscattering term $\mathbf{H}_t^u\boldsymbol{\phi}^{n-1}$ in Eq. (A.10) is replaced by $\mathbf{H}_t^u\boldsymbol{\phi}^n$; this requires repetitive iterations in the thermal groups.[169]

There are several alternatives for the solution of the in-group source problem. For small-matrix problems, such as small one-dimensional cell calculations, the solution is obtained by direct inversion.[134,169] For larger size problems, a power iteration technique and successive overrelaxation are applied.[115,128,169]

The power iteration method is formally equivalent to the multiple scattering formalism for the solution of the integral equation.[205] Power iterations also can be accelerated by using the residual minimization technique. To describe this method, we consider the power iteration solution of Eq. (A.11), which we write as

$$\boldsymbol{\phi}^k = \mathcal{L}\boldsymbol{\phi}^{k-1} + \boldsymbol{Q} \ , \qquad \text{(A.12)}$$

where k is the inner iteration index and $\mathcal{L}$ represents the operator $\mathbf{G}\boldsymbol{\Sigma}_{s0}$. At any stage of iteration, the remainder may be defined as

$$\boldsymbol{\epsilon}^k = \boldsymbol{\phi}^k - (\mathcal{L}\boldsymbol{\phi}^k + \boldsymbol{Q}) \ .$$

Then the iteration procedure is defined as

$$\boldsymbol{\phi}^k = \boldsymbol{\phi}^{k-1} + \alpha^{k-1}\boldsymbol{\epsilon}^{k-1} \ , \qquad \text{(A.13)}$$

where the acceleration parameter α^{k-1} is chosen so that the remainder $\boldsymbol{\epsilon}^k$ is minimized.

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[204]E. M. GELBARD and L. A. HAGEMAN, *Nucl. Sci. Eng.*, **37**, 288 (1969).

[205]D. E. CULLEN, *Nucl. Sci. Eng.*, **53**, 93 (1974).

The entire residual minimization acceleration requires three vectors, and may be summarized by the following procedure: Starting with the previous values ϕ^{k-1} and ϵ^{k-1}, we compute the intermediate vector $\tilde{\phi}^k$,

$$\tilde{\phi}^k = (\mathbf{I} - \mathcal{L})\epsilon^{k-1}$$

and calculate the acceleration parameter

$$\alpha^{k-1} = -(\tilde{\phi}^k, \epsilon^{k-1})/(\tilde{\phi}^k, \tilde{\phi}^k) \ ,$$

where (,) denotes an appropriate scalar product. For instance,

$$(\boldsymbol{a},\boldsymbol{b}) = \sum_i V_i a_i b_i \ ,$$

where i denotes the zone index. Finally, the new flux is calculated from Eq. (A.13) and the new remainder is obtained from

$$\epsilon^k = \epsilon^{k-1} + \alpha^{k-1}\tilde{\phi}^k \ .$$

In usual practice, best results are obtained by alternating power iterations with residual minimization accelerations.[169]

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